Thesis for the degree of Licentiate of Engineering

Novel Approaches for Retrofitting Heat Exchanger Networks Subject to Varying Operating Conditions

CHRISTIAN LANGNER

CHALMERS
UNIVERSITY OF TECHNOLOGY

Department of Space, Earth and Environment
Division of Energy Technology
Chalmers University of Technology
Gothenburg, Sweden 2020

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CHRISTIAN LANGNER

Department of Space, Earth and Environment
Division of Energy Technology
Chalmers University of Technology
SE-412 96 Gothenburg
Telephone +46 31 772 1000

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Christian Langner
Department of Space, Earth and Environment
Chalmers University of Technology

Abstract

The process industry is responsible for a significant share of the final industrial energy use in Sweden. In particular, the pulp and paper industry accounts for more than 50 %. In this context, a number of studies have shown that there is a substantial potential for energy savings in the pulp and paper industry. In particular, increased heat recovery is an important measure for increasing energy efficiency. Industrial process plants usually include heat recovery systems that are built to transfer heat between different process streams. Such heat recovery systems consist of Heat Exchanger Networks (HENs) which can be characterized by a high degree of complexity, e.g. through stream splits, recycle and closed circulation loops.

Increasing heat recovery, e.g. by redesigning (retrofitting) the existing heat recovery system, can contribute significantly to meeting energy efficiency improvement targets for industrial process plants. One issue to consider when screening retrofit design options is that industrial heat recovery systems must be able to handle external variations, e.g. in inlet temperatures or heat capacity flow rates, in such a way that operational targets are reached. Consequently, there is a need for systematic retrofitting methodologies applicable to HENs subject to variation in operating conditions. The aim of this thesis is to propose new approaches for retrofitting HENs operating in multiple periods.

Three different approaches have been developed and published in three papers appended to this thesis which allow for retrofitting HENs operating in multiple periods. These approaches can be applied independently and are applicable to HENs commonly present in process industry, e.g. pulp and paper industry. All approaches have in common that they require structural retrofit design proposals as input. For the structural proposal generation, graphical approaches (e.g. Pinch-based) may be utilized in order to take advantage of the designer interaction during the design process. The three approaches propose different strategies to evaluate and ensure feasibility of the design proposals when operating conditions vary, e.g. by means of design modifications. In this context, feasibility is achieved if predefined target values, e.g. stream target temperatures, can be reached for the entire span of variations. Furthermore, different strategies help the designer to identify the most promising proposal (or proposals) among the provided ones with respect to a defined objective, e.g. most energy-efficient or most cost-efficient.

Keywords: Heat Integration; Retrofit; Multi-Period Optimization; Process Industry; Critical Points; Flexibility; Feasibility; Energy Efficiency.

List of Publications

The following papers are included in this thesis:

Paper I: C. Langner, E. Svensson, and S. Harvey, "A computational tool for guiding retrofit projects of industrial heat recovery systems subject to variation in operating conditions", submitted to Applied Thermal Engineering, March 2020.

Paper II: C. Langner, E. Svensson, and S. Harvey, "Combined Flexibility and Energy Analysis of Retrofit Actions for Heat Exchanger Networks", Chemical Engineering Transactions, vol. 76, pp. 307–312, 2019, doi: 10.3303/CET1976052.

Paper III: C. Langner, E. Svensson, and S. Harvey, "A Framework for Flexible and Cost-Efficient Retrofit Measures of Heat Exchanger Networks", Energies, vol. 13, paper no. 1472, 2020, doi: 10.3390/en13061472.

Co-authorship statement

Christian Langner (CL) is the main author for all papers included in the thesis. Elin Svensson (ES) and Simon Harvey (SH) supervised the work and provided critical feedback on all paper draft manuscripts. CL, ES and SH discussed the research continuously during the work for all papers included in the thesis. The tool appended to Paper I as supporting material was developed by Pontus Bokinge (PB) and David Erlandsson (DE) who also collected process data used for the case study (in Paper I).

Related papers not included in this thesis:

C. Langner, E. Svensson, P. Bokinge, D. Erlandsson, and S. Harvey, "A computational tool for analysing the response of complex heat exchanger networks to disturbances," in Proceedings of the 29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems, 2019, pp. 621–633.

E. Svensson, R. Edland, C. Langner, and S. Harvey, "Assessing the value of a diversified by-product portfolio to allow for increased production flexibility in pulp mills", submitted to Nordic Pulp & Paper Research Journal, April 2020.

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Christian Langner, Gothenburg, April 2020

Contents

List of Figures

List of Tables

1
Introduction

In 2020, humanity faced the global outbreak of the pandemic virus Sars-CoV-2. In this context, the so called "flattening the curve" concept was omnipresent in media to sensitize general public to the capacity limit of the public health care sector. With increasing media presence of the "flattening the curve" concept, popular science media started using the concept to raise awareness of the increase of the global average temperature (see, e.g. [3–5]). While prior to the outbreak of Sars-CoV-2, "flattening the curve" would have raised question-marks in the general public, the concept could now be related to restrictive measures to control the speed (gradient) of a time-dependent development. In the terms of climate change, the annual global greenhouse gas emissions have been increasing steadily since early industrialization and are projected to increase even further if not restricted by counter-measures. There is a widespread consensus among scientists that the capacity limit of the earth's ecosystems has already been reached (if not exceeded) and that restrictive measures can contribute to avoiding too severe damage to sensitive ecosystems. The main effect of the increasing greenhouse gas emissions has been the raise of the global average temperature. Different scenarios project the future development of the global average temperature depending on the projected global greenhouse gas emissions (see, e.g. Figure 1). As indicated in Figure 1, political decisions have a major influence on the projected global greenhouse gas emissions. In this context, political initiatives, such as the Paris Agreement in 2015 [6], have agreed on the necessity to limit the maximum increase of the global average temperature compared to pre-industrial measurements. Figure 1 shows which substantial decreases of global greenhouse gas emissions are necessary if different limits for the maximum increase of the global average temperature are pursued. It should be noted that already in 2015, the phrase "bending the curve" was used by Ramanathan et al. [7] to describe different scenarios for how to limit the increase rate of the global average temperature.

As mentioned above, several political initiatives such as the Paris Agreement [6] or the European 2030 Climate and Energy framework [8] stress the urgency of measures to limit the raise of the global average temperature. In this context, increased energy efficiency can be interpreted as one of the key-measures. Figure 2 shows the potential of different measures for reducing the annual global CO_2 emissions in the energy sector to reach a sustainable development scenario developed by the International Energy Agency (IEA) [2]. It should be noted that the energy sector is responsible for more than 70 % of the annual global CO_2 emissions [9]. According to the IEA, increased energy efficiency can contribute the most to reducing the annual global CO_2 emissions in the energy sector (compare Figure 2). Furthermore, the European Union (EU) formulated its own directive for increasing energy efficiency in 2012 [10]. In 2018, an amendment to the EU's Directive on Energy Efficiency was formulated by the European Commission in which the member states are required to increase the efficiency of final energy use by 32.5 % by 2030, compared to

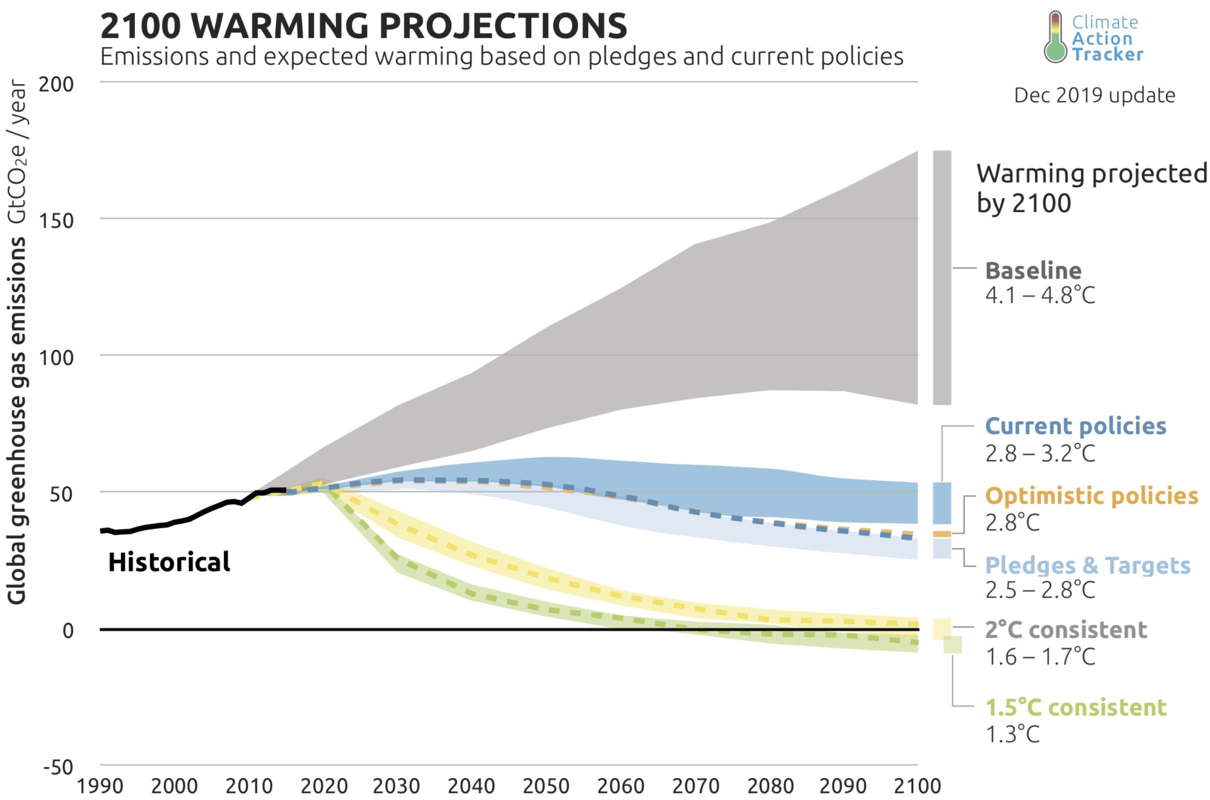


Figure 1: Different projections of the annual global greenhouse gas emissions and the resulting raise of the global average temperature in comparison to pre-industrial measurements. [1]

2007 [11]. In Sweden, national targets have been formulated that take the economic development into account, and the national energy agency has been commissioned by the government to ensure a reduction in energy intensity (primary energy consumption per unit of GDP) by 50 % by 2030, compared to 2005 [12]. In 2017, the total Swedish final energy use was reported to be 378 TWh of which 143 TWh in industry [12]. The process industry was responsible for a significant share of the final industrial energy use in Sweden, and especially the pulp and paper industry which accounted for more than 50 % must be mentioned [12]. For increasing the energy efficiency in the pulp and paper industry, increased heat recovery is one important measure that has been suggested in numerous studies found in the literature, e.g. [13–22]. To increase heat recovery in an existing plant, retrofitting of the heat recovery system in place is usually necessary.

Industrial heat recovery systems often consist of large and complex Heat Exchanger Networks (HENs) to transfer heat between different process streams. For example, in pulp and paper mills, secondary heating systems may be in place as a complement to direct process-to-process heat exchange. In these secondary heating systems, a heat transfer medium (commonly water) is used to recover/distribute heat from/to primary process streams, in order to avoid operability issues resulting from the direct interconnection of different process streams. The interconnections between the secondary heating system and the primary processes are commonly characterized by a high degree of complexity, e.g. through stream splits, recycle and closed circulation loops. Additionally, there are commonly high demands on the reliability of industrial heat recovery systems as heating

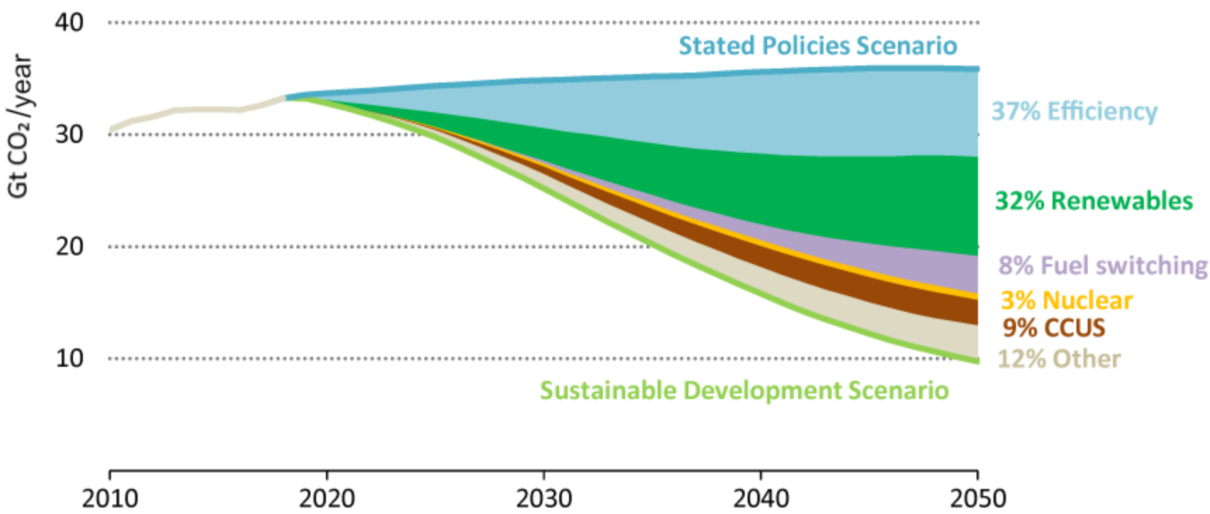


Figure 2: Potential of different measures to reduce the annual global greenhouse gas emissions in the energy sector to reach a sustainable development scenario developed by the International Energy Agency. [2]

and cooling capacity is essential for the operability of the core production process. Further challenges when planning for retrofitting of industrial heat recovery systems are availability and reliability of measured data as well as interdependencies and correlations within this data. Finally, one should mention the difficulties identifying appropriate cost data necessary to estimate the costs of making changes to existing equipment. Consequently, retrofitting methodologies which should be applicable to industrial heat recovery systems must be able to handle this high degree of complexity and the specific characteristics of these systems.

1.1 Literature Review

Systematic approaches to design heat recovery systems, especially HENs, have been subject to a substantial volume of research since the early 1980s with the introduction of the graphical Pinch analysis method [23]. In addition to the graphical Pinch analysis method, mathematical programming is a well-established complementary approach to HEN synthesis. Both sequential approaches [24] and simultaneous approaches [25], where targeting and network synthesis are performed separately and simultaneously, respectively, have been developed and reported in the literature. In addition, hybrid methods, which combine graphical methods and mathematical programming [26], have been suggested. Both graphical and mathematical methods for the design of heat recovery systems have been further developed and are well-established, and an overview as well as a comparison on different methods can be found in [27].

Compared to the synthesis of HENs for greenfield problems, the rearrangement of an existing HEN (retrofitting) is a different problem. In contrast to greenfield design situations, a retrofitting problem is often characterized by additional constraints and limitations resulting in highly individual problems. Extensive work exists on retrofitting methodologies based on graphical insights (e.g. Lai et al. [28], Kamel et al. [29], Bonhivers et al. [30]), mathematical programming (e.g. Ciric and Floudas [31], Asante and Zhu [32], Athier et al. [33]), and those methodologies that can be characterized as hybrid methodologies combining graphical analysis and mathematical programming (e.g. Smith et al. [34], Jiang et al. [35], Akpomiemie and Smith [36]). A comprehensive overview of different retrofitting methodologies can be found in [37].

The above-mentioned retrofit methodologies for HENs do not account for variations and uncertainties in operating data, e.g. in inlet temperatures or heat capacity flow rates. Usually, steady-state or average values are considered (see above), i.e. the reported methodologies can only be applied to single-period models of HENs. However, industrial plants are subjected to different kinds of time-dependent variations [15]. These variations can occur on very different timescales and are often characterized as short-, medium- or long-term variations [15]. Variations in the short term usually relate to disturbances in the process. These disturbances can have various reasons and one example is the daily variation of the ambient air temperature. In comparison to short-term variations, variations in the medium term relate to seasonal changes. In the case of long-term variations, an example is changes in legislation which can affect strategic business decisions and result in operational adjustments but also in changes of the plant's process configuration.

Persson and Berntsson [15] showed that considering annual average values to calculate the steam savings potential of a retrofit heat integration project in a pulp mill can lead to an overestimation of 15 % compared to the steam savings potential calculated with monthly average values. Persson and Berntsson further concluded in [38] that the steam savings potential decreases even further if it is calculated with average values of shorter time periods (e.g. daily or 10-min periods). In contrast to the results reported by Persson and Berntsson as well as the excessive amount of methodologies available for retrofitting single-period models of HENs, very little published literature relates to retrofitting HENs which are subject to variations in operating conditions. Papalexandri et al. [39] developed a multi-period Mixed Integer (Non-)Linear Program (MI(N)LP) model, which is based on multi-period hyperstructures which include all considered retrofit proposals. Furthermore, Papalexandri et al. [39] proposed an iterative scheme between the developed multi-period MI(N)LP and a flexibility analysis sub-problem. The aim is to identify the retrofit proposal that yields the minimum total annualized cost and is operable for predefined variations. Another retrofitting methodology was reported by Kang and Liu [40], who introduced a two-step method to identify retrofit design proposals that can operate cost-efficiently in multiple periods. In the first step, the multi-period HEN synthesis model is used, as in greenfield design problems (see, e.g. [41]). In the second step, existing exchangers are relocated in order to meet the required area demands identified in step one, i.e. eliminate existing area mismatches.

Although the above-mentioned retrofit approaches (i.e. [39, 40]) account for variations and uncertainty in operating data, there are several reasons why these approaches are not easily applied to large and complex industrial applications. As mentioned previously, complexities, such as splitting or re-circulation of streams, are commonly present in industrial heat recovery systems. These complexities cause non-linearities in the mathematical formulation of these systems which inevitably leads to difficulties in finding feasible solutions for the resulting multi-period MINLP formulation proposed in [39]. A further difficulty arising with the approach of Papalexandri et al. [39] is that the flexibility analysis sub-problem can be difficult to solve for large and complex industrial applications even with state-of-the-art global MINLP solvers. Moreover, depending on the problem complexity itself, the solution produced by common multi-period HEN synthesis formulations and the current network layout may differ significantly. Consequently, relocating existing exchangers to meet identified area requirements as proposed in [40] can easily result in inefficient trial and error procedures.

The above reported methodologies (i.e. [39,40]) are based on mathematical programming, which is a powerful approach when dealing with variations in operating data. However, in comparison to these methodologies, graphical methods have great potential to be applied to large and complex applications due to their beneficial user interaction. Different strategies have been reported in the literature to utilize approaches based on graphical insights in the design process of multi-period HEN retrofitting case studies. A common strategy to deal with variations in operating conditions from a Pinch analysis perspective is to develop different retrofit proposals for a number of selected sets of operating conditions (e.g. annual, seasonal or monthly average values) [15]. The different design proposals are then evaluated and may be combined to achieve an operable and energy-efficient retrofit proposal, accounting for all considered operating points. Another strategy is to develop different retrofit proposals by applying a graphical retrofitting methodology (e.g. methodologies based on temperature driving force curves [29] or identifying retrofit bridges [30]) for a specific nominal point and analyze the network's response to variations in a separate analysis step. Recently, Lal et al. [42] applied this approach to obtain insights and to identify the best performing retrofit design proposal by means of Monte Carlo simulation. However, neither Persson and Berntsson [15] nor Lal et al. [42] thoroughly explored the adjustment of operational degrees of freedom in a HEN, e.g. split ratios or bypass ratios. These operational degrees of freedom can be adjusted to maintain operability (e.g. stream target temperatures) when variations in operating data occur. To investigate the influence of such adjustments, optimization or (additional) trial-and-error calculations would have been necessary. In conclusion, approaching a retrofit problem subject to variations in operating data from a graphical analysis perspective relies to a large extent on time-consuming procedures since different design proposals must be evaluated and manually combined. Good results can be obtained, but the design process itself is often very inefficient due to the trial-and-error character of the respective strategies.

In summary, systematic methodologies for retrofitting industrial HENs subject to variation in operating data are needed, but the available methodologies fulfill this demand only partly. Apart from the fact that industrial heat recovery systems usually have very complex structures, a common issue is that retrofitting problems are more constrained due to already existing equipment which leads to very complex and individual problems.

1.2 Aim

To overcome the above-mentioned shortcomings of available retrofitting methodologies, this thesis aims to propose new approaches for retrofitting HENs operating in multiple periods. Three different approaches have been developed and published in three papers appended to this thesis which allow for retrofitting HENs operating in multiple periods. These approaches can be applied independently and are applicable to HENs commonly present in process industry, e.g. pulp and paper industry. Furthermore, the thesis investigates to what extent tools and strategies specifically developed for pursing one of these approaches can be utilized in one of the other two approaches. This is achieved by presenting the theoretical concepts upon which the different approaches are based, followed by a presentation of the approaches. The developed approaches have in common that they require structural retrofit design proposals as input. For the structural proposal generation, graphical methodologies (e.g. Pinch-based) may be utilized in order to take advantage of the designer interaction during the design process. The three approaches propose different strategies to evaluate and ensure feasibility of the (input) design proposals when operating conditions vary, e.g. by means of design modifications. In this context, feasibility is achieved if predefined target values, e.g. stream target temperatures, can be reached for the entire span of variations. Furthermore, different strategies are proposed to help the designer to identify the most promising proposal (or proposals) among the provided ones with respect to a defined objective, e.g. most energy-efficient or most cost-efficient.

1.3 Appended Papers

A general idea followed in the development of the three approaches was to reduce the complexity of the overall retrofitting problem by dividing the retrofitting process into several sub-steps. This allows, for example, to combine the beneficial designer interaction of graphical methodologies with the efficiency of mathematical programming. Different strategies are utilized in the developed approaches to achieve retrofit solutions which are feasible but also energy-efficient and/or cost-efficient for the entire operating range. As mentioned previously, all approaches have in common that they require structural retrofit design proposals as input. The approaches are presented in three different papers appended to this thesis:

- Paper I: C. Langner, E. Svensson, and S. Harvey, “A computational tool for guiding retrofit projects of industrial heat recovery systems subject to variation in operating conditions”, submitted to Applied Thermal Engineering, March 2020;
- Paper II: C. Langner, E. Svensson, and S. Harvey, “Combined Flexibility and Energy Analysis of Retrofit Actions for Heat Exchanger Networks”, Chemical Engineering Transactions, vol. 76, pp. 307–312, 2019, doi: 10.3303/CET1976052; and
- Paper III: C. Langner, E. Svensson, and S. Harvey, “A Framework for Flexible and Cost-Efficient Retrofit Measures of Heat Exchanger Networks”, Energies, vol. 13, paper no. 1472, 2020, doi: 10.3390/en13061472.

In Paper I, a computational analysis tool is proposed which enables fast evaluation of the HEN’s response, i.e. temperatures and heat loads, when operating conditions change and/or operational settings are manipulated. Additionally, a strategy is outlined to automatically derive the complete set of equations necessary to describe the heat and mass balances of a given HEN. The proposed strategy is applicable for a wide range of HEN structures (including common complexities such as re-circulating streams). The computational analysis tool can be used to screen previously generated HEN retrofit design proposals, and a systematic methodology is presented for applying the analysis tool in retrofitting design processes to evaluate the operability and performance of different retrofit design proposals for the entire operating period by means of sensitivity analysis. The proposed methodology is applied in Paper I to compare different Pinch-based retrofit proposals for a subsystem of the secondary heating system of a large modern Kraft pulp mill.

In Paper II, it is proposed to evaluate the previously generated design proposals in an analysis step in which the initial set of designs is narrowed down to one or several design options that are operable and energy-efficient for predefined variations of operating conditions. Traditional feasibility assessment of HENs (i.e. the calculation of the flexibility index) to identify structurally infeasible design proposals is combined with energy performance analysis. Additionally, a trial-and-error approach is proposed to identify feasible design characteristics of structurally feasible design proposals. The proposed approach is illustrated by means of a HEN case study.

In Paper III, a framework is proposed which divides the retrofitting processes into five sub-steps. In a first step, the previously generated design proposals are incorporated into a superstructure. By means of feasibility assessment, structurally infeasible design proposals are identified and can be discarded from further analysis, yielding a reduced superstructure. Additionally, critical point analysis is applied to identify those operating points within the uncertainty span that require necessary oversizing of heat exchangers. In the final step, the most cost-efficient design proposal within the reduced superstructure is identified by means of multi-period optimization. The proposed framework is applied to a HEN retrofit case study to illustrate the five sub-steps.

In Figure 3, an overview on the appended papers is provided. Additionally, the main strategies which have been utilized in the papers are highlighted.

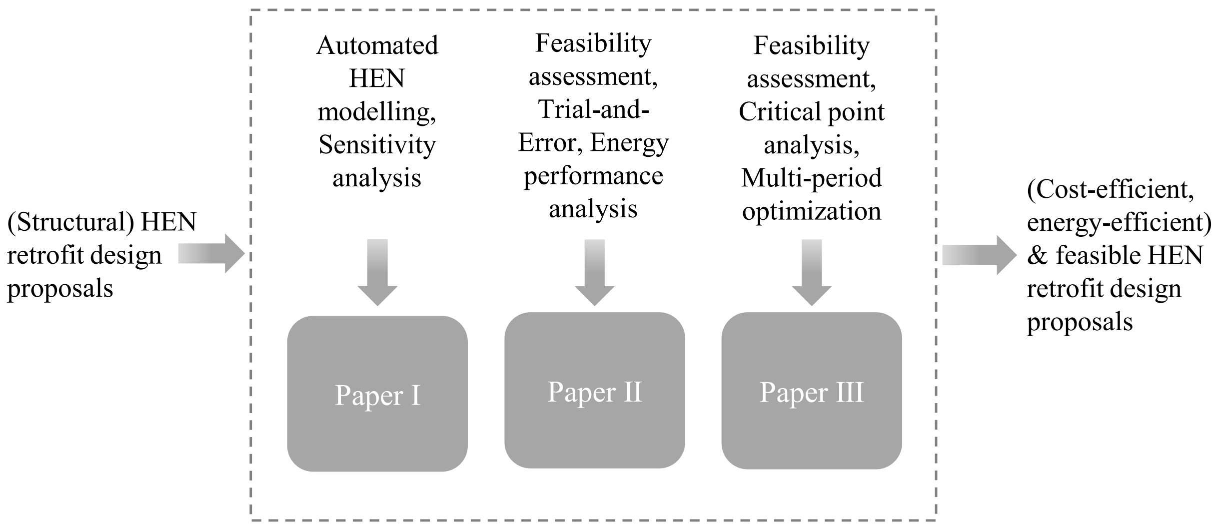


Figure 3: Overview of appended papers.

2

Theoretical background

This chapter presents the theoretical background of the three approaches to achieve feasible and cost-efficient/energy-efficient retrofit measures which are outlined in Chapter 3. The concepts and assessment methodologies introduced are utilized in the different approaches. If applicable, the literature regarding a certain concept is reviewed and summarized. The concepts introduced in this chapter are:

- Heat Exchanger Network Response;
- Heat Exchanger Network Modelling;
- Feasibility Assessment of Heat Exchanger Networks - Flexibility Index;
- Multi-Period Optimization; and
- Critical Point Analysis.

2.1 Heat Exchanger Network Response

A Heat Exchanger Network (HEN) is usually characterized by a number of fluid streams which interchange heat by means of Heat Exchangers (HEXs). The heat exchange can be direct or indirect (i.e. by means of a heat transfer medium). A typical graphical representation of a HEN is the grid diagram, as illustrated in Figure 4.

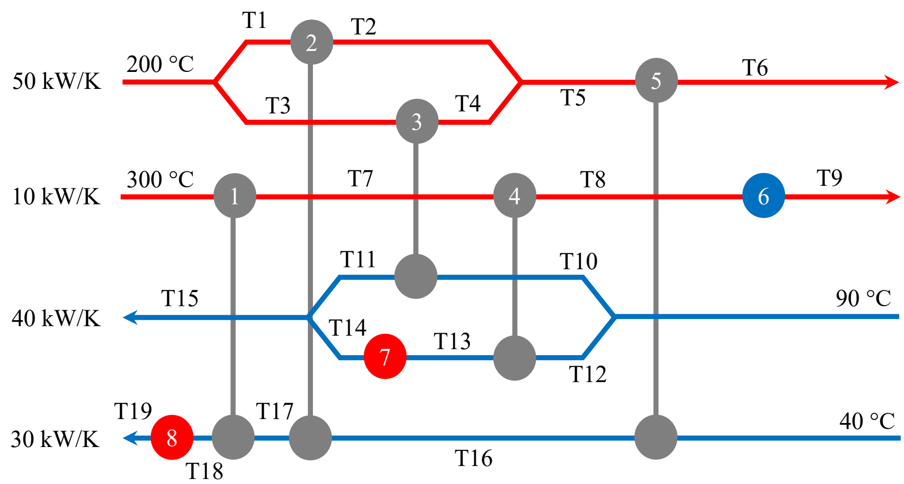


Figure 4: An example heat exchanger network in the grid representation illustrating the (unknown) network temperatures.

In Figure 4, the (unknown) network temperatures are marked. The network temperatures describe the temperature change over the different streams due to heat exchange in

HEXs, stream splits and mixing of streams. This implies that the number of (unknown) network temperatures for a fixed HEN structure can be calculated a priori [43]. For a network with N streams, n_E process-to-process HEXs, n_S stream splits (1 stream splits into 2 streams), n_M stream mixing points and n_U utility HEXs, the number of (unknown) network temperatures N_T is:

$$N_T = N + 2 \cdot n_E + 2 \cdot n_S + n_M + n_U. \tag{2.1}$$

The number of (unknown) temperatures N_T is reduced by N if the supply temperatures for all streams are specified. For the example HEN shown in Figure 4, the following information is given:

- Four (main) streams with a specified supply temperature;
- Five process-to-process HEXs;
- Two stream splits;
- Two stream mixing points; and
- Three utility HEXs.

According to Equation 2.1, the number of (unknown) network temperatures is 23 of which four are known since the supply temperatures of the streams are specified. Therefore, the number of (unknown) network temperatures is 19 which agrees with the marked temperatures in Figure 4.

The network response of a HEN usually refers to the network temperatures (see, e.g. [44] and [45]). This means that the network response may change if operating conditions change, e.g. supply temperatures, heat capacity flow rates and heat transfer coefficients. If the network response of a HEN changes, operability and energy utility requirements of the HEN are affected. In this context, the operability of a HEN is commonly defined by the ability to maintain operating constraints, e.g. fixed (or desired) target temperatures for all relevant streams. An unwanted network response, e.g. operability issues or increased energy demand, can (sometimes) be avoided or minimized by means of manipulations of operational parameters or degrees of freedom such as split ratios or HEX bypass ratios. The network response can be calculated for a fixed set of operating conditions and operational parameters by means of a mathematical HEN model which is presented in Section 2.2.

In this thesis, in addition to the network temperatures, the response of a HEN includes the internal heat capacity flow rates which result from splitting and mixing of streams as well as the loads of (utility) HEXs (i.e. heaters and coolers). The latter is of special interest when evaluating the energy efficiency of a HEN since the energy efficiency of a HEN is assessed by the need for external heating and cooling utilities.

2.2 Heat Exchanger Network Modelling

Mathematical modelling of HENs is necessary for several purposes, e.g. calculation of the network response (see Section 2.1) but also calculation of the flexibility index (see Section

2.3) or identification of the most cost-efficient design characteristics (see Section 2.4). A mathematical model of a HEN consists of the following set of equations:

$$h_i(d, x, z, \Theta) = 0;\ i \in I, \tag{2.2a}$$

$$g_j(d, x, z, \Theta) \leq 0;\ j \in J, \tag{2.2b}$$

where d is the vector of design variables, x corresponds to the state variables, z is used for the control variables and the inlet conditions or uncertain parameters are depicted by Θ. In HENs, typical design variables are the area values of HEXs, while typical uncertain parameters are inlet temperatures or heat capacity flow rates of process and/or utility streams. State and control variables correspond to network temperatures and duties of HEXs. In the mathematical sense, the difference between state and control variables is that state variables are determined by means of the equality constraints $i \in I$ while control variables are degrees of freedom. The nature of the set of equations depends on the physical components present in the HEN. Common physical components are:

- Heat Exchangers (HEXs):
  - direct process-to-process HEXs;
  - indirect process-to-(heat transfer medium) HEXs;
  - utility HEXs (e.g. steam heaters or coolers);
- Splitters; and
- Mixers.

Other physical components such as reactors can be found in HENs, but these components were not be considered explicitly in this thesis. On the other hand, components such as reactors can be modeled implicitly by means of identity changes of process streams. Switch models were used to model these identity changes of process streams and further explanation can be found in Subsection 2.2.3.

2.2.1 Heat Exchanger Modelling

A common approach to model HEXs in HENs is formulating energy balances on the hot and cold stream side of each HEX. Additionally, heat transport equations are used to account for the design characteristics of a HEX since the heat exchange in a HEX is constrained by the available surface area. This is formulated in Equations 2.3a to 2.3c:

$$Q_{HEX} = CP_h \cdot (T_{h,in} - T_{h,out}), \tag{2.3a}$$

$$Q_{HEX} = CP_c \cdot (T_{c,out} - T_{c,in}), \tag{2.3b}$$

$$Q_{HEX} = U_{HEX} \cdot A_{HEX} \cdot \Delta T_{LM}. \tag{2.3c}$$

In Equations 2.3a to 2.3c, the index h is used for hot process (or secondary) streams and the index c is used for cold process (or secondary) streams. Consequently, Q_{HEX} is positive if heat is transferred from the hot stream to the cold stream connected by means of the HEX. In several mathematical HEN models, this is an additional constraint (i.e. $Q_{HEX} \geq 0$).

In industrial HENs, bypasses are usually available around HEXs for control purposes. These bypasses can be modeled explicitly (see, e.g. Appendix B.1 of [46]). However, as explicit modelling introduces additional non-linearities, alternative modeling approaches have been investigated. One possibility commonly found in the literature (e.g. in [47]) is to relax the equality sign in Equation 2.3c by a less or equal sign ($\leq$) for those HEXs which feature a bypass. This way, it is assumed that the effective area of a HEX can be smaller than the installed area which gives a similar result as a bypass. Additionally, physical operating constraints for the temperatures must be defined. For a counter-current HEX, these operating constraints are given in Equations 2.4a and 2.4b:

$$T_{h,in} - T_{c,out} \geq \Delta T_{min}, \tag{2.4a}$$

$$T_{h,out} - T_{c,in} \geq \Delta T_{min}. \tag{2.4b}$$

In Equations 2.4a and 2.4b, ΔT_{min} must be larger or equal to 0 if heat is transferred from the hot to the cold stream. Additionally, in comparison to available mathematical HEN models in the literature, in this thesis it was considered that Equations 2.4a and 2.4b cannot be evaluated independently of Equations 2.3a to 2.3c. If, for example, a HEX is entirely bypassed (i.e. $Q_{HEX} = 0$), the physical operating constraints 2.4a and 2.4b must not be strictly obeyed as the HEX is out of operation. In order to model this mathematically, Equations 2.4a and 2.4b can be multiplied by the temperature difference on the right-hand side of either Equation 2.3a or Equation 2.3b. This way, it is ensured that the physical operating constraints only are meaningful if the HEX is transferring heat.

In order to model specific HEX types such as shell-and-tube HEXs or plate HEXs, standard methods such as the P-NTU method (a variation of the ϵ-NTU method) can be used. The P-NTU method is based on the thermal effectiveness (P) of a HEX. P is individually defined for the hot (index h) and the cold (index c) stream side of the HEX:

$$P_h = \frac{T_{h,in} - T_{h,out}}{T_{h,in} - T_{c,in}}, \tag{2.5a}$$

$$P_c = \frac{T_{c,out} - T_{c,in}}{T_{h,in} - T_{c,in}}. \tag{2.5b}$$

The denominator is the same for both definitions and represents the maximum possible temperature change for any of the fluids in the HEX. For different HEX types, closed form expressions, which are based on experimental data, to calculate P are defined, e.g. in [48, 49]. Generally, these closed form expressions for P have the following form:

$$P_i = f(NTU_i\ ,\ R_i\ ,\ \text{flow arrangement}\ ,\ \text{fluid allocation}), \tag{2.6a}$$

$$NTU_i = UA/CP_i, \tag{2.6b}$$

$$R_i = CP_i/CP_{\neq i}, \tag{2.6c}$$

where i is h for the hot stream side or c for the cold stream side. Consequently, for given UA and CP_i values, P can be calculated independently of the actual temperatures which means that the unknown outlet temperatures $T_{h,out}$ and $T_{c,out}$ can be calculated using Equations 2.5a and 2.5b (assuming that the two inlet temperatures $T_{h,in}$ and $T_{c,in}$ are known).

In industrial applications, heat exchange can happen due to non-isothermal mixing. A common example is steam injection in order to heat a process stream to its final target temperature. In these or similar cases, the heat exchange is neither limited by heat transfer area nor is any measurable heat transfer area present. It is possible to describe the steam injection mathematically as a mixing process and therefore by means of energy and mass balances (see Subsection 2.2.2). However, the heat which is transferred in these cases can also be derived by a single energy balance around the process stream since both inlet and outlet (i.e. fixed target) temperature are known. This way of modelling may also be practical for (other) utility HEXs since usually utility HEXs are oversized to guarantee operability and the transferred heat is the interesting physical quantity to be determined by modelling.

2.2.2 Modelling of Stream Splitting and Mixing

Besides HEXs, splitters and mixers are components commonly present in HENs. In the example HEN shown in Figure 4, two stream splits and two mixing points are present. To model stream splitting and mixing, energy and mass balances are important to consider. In the case of stream splitting, isothermal splitting can usually be assumed. Therefore, for a split of one stream into n streams, the energy balance can be simplified:

$$T_{out,1} = T_{out,n} = T_{in}. \tag{2.7}$$

The mass balance for a split of one stream into n streams is:

$$\sum_{i=1}^{n} \dot{m}_{out,i} = \dot{m}_{in}. \tag{2.8}$$

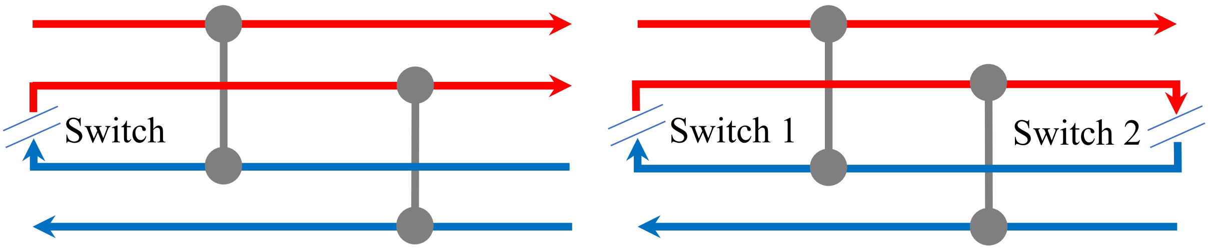
In the case of mixing n input streams to one output stream, mass and energy balances are given in the following:

$$\sum_{i=1}^{n} (\dot{m}_{in,i} \cdot cp_{in,i} \cdot T_{in,i}) = \dot{m}_{out} \cdot cp_{out} \cdot T_{out}, \tag{2.9a}$$

$$\sum_{i=1}^{n} \dot{m}_{in,i} = \dot{m}_{out}. \tag{2.9b}$$

2.2.3 Modelling of Identity Changes

In this thesis, the identity of a stream is defined by whether the stream releases heat (hot stream) or receives heat (cold stream) in the HEXs on the stream. Consequently, an identity change implies that a stream changes from being identified as cold to hot or vice versa. These identity changes may occur in (industrial) HENs, e.g. when streams are re-circulated or in closed circulation loops. Figure 5 visualizes the identity change of a) a re-circulating stream and b) a closed circulation loop by means of switches. In order to model an identity change, one solution is to model a new stream for each identity change. However, inlet conditions to these new streams are defined by the conditions prior to the identity change (see Figure 5). Therefore, trivial pairs of equations describing the relation between the temperatures ($T_{out,c}$ and $T_{in,c}$) as well as the CP-values ($CP_{out,c}$ and $CP_{in,c}$) over the identity change $c \in IC$ can be derived. Another example for an identity change is an endothermic reactor since reactor feed needs to be heated (cold stream) while it is usually possible to recover some heat from reactor outlet streams (hot stream).



(a) Identity change in a re-circulating stream

(b) Identity changes in a closed circulation loop

Figure 5: Visualization of the identity change of a stream (i.e. a hot stream becomes a cold stream or vice versa).

2.3 Feasibility Assessment of Heat Exchanger Networks - Flexibility Index

In this section, the flexibility index as a concept for performing feasibility assessment of HENs is briefly introduced. For further information, the reader is referred to the literature references listed in this section.

Flexibility analysis of HENs has been subject to research since the early 1980s. In 1982, Marselle et al. [50] first introduced the concept of resilient HENs with respect to a certain disturbance range in the inlet conditions. In 1985, Saboo et al. [51] introduced a resilience index to quantify the resilience of HENs. In the same year, Swaney and Grossmann [52] extended the concept of the resilience index to a flexibility index which is applicable not only to HENs but also to chemical processes in general. Both the resilience and the flexibility index indicate the maximum disturbance range in which inlet conditions may vary while at the same time achieving feasible operation. This maximum disturbance range can be interpreted as a hyperrectangle (multi-dimensional rectangle, e.g. cuboid for three dimensions) in the space of the varying inlet conditions. In this context, both indices are defined as the ratio between the largest scaled hyperrectangle within the feasible region and the hyperrectangle defined by an expected disturbance range. Therefore, feasibility is achieved if the respective index is larger or equal to 1. For two varying inlet conditions this can be visualized as in Figure 6. For the example shown in the figure, the largest scaled rectangle within the feasible region can be expressed mathematically by the following set of equations (δ corresponds to the flexibility/resilience index):

$$T_{1,N} - \delta \cdot \Delta T_1^- \leq T_1 \leq T_{1,N} + \delta \cdot \Delta T_1^+, \tag{2.10a}$$

$$T_{2,N} - \delta \cdot \Delta T_2^- \leq T_2 \leq T_{2,N} + \delta \cdot \Delta T_2^+. \tag{2.10b}$$

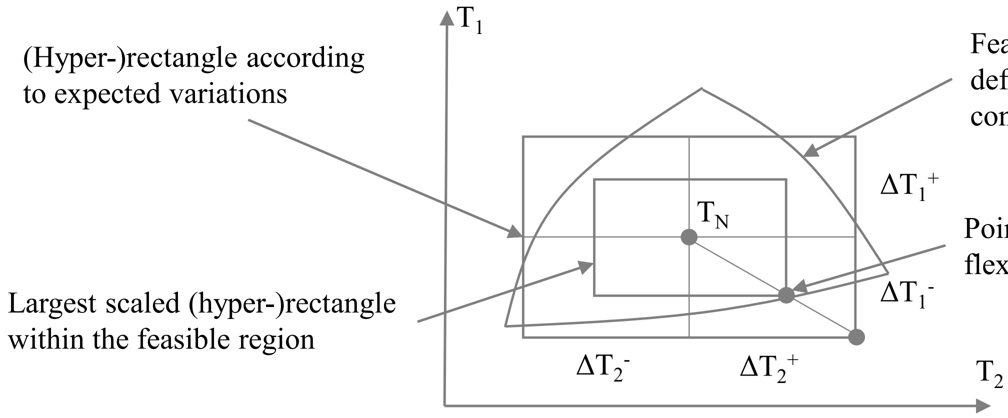


Figure 6: Visualization of the flexibility index: (Hyper-)rectangle with respect to expected variations and maximum scaled (hyper-)rectangle inscribed within the feasible region in the space of the varying inlet temperatures of a heat exchanger network.

In Figure 6, the largest scaled rectangle within the feasible region is smaller than the rectangle corresponding to the expected variations. Thus, feasibility with respect to the expected variations is not achieved (flexibility or resilience index is smaller than 1). Feasibility is achieved when all constraints $i \in I$ and $j \in J$ (compare 2.2a and 2.2b) are satisfied at the point of operation. With both formulations, it is possible to describe the resilience or feasibility for convex problems in which the solution lies at a vertex point of the largest scaled (hyper-)rectangle within the feasible region (see Figure 6). In 1987, Grossmann and Floudas [53] developed an active set approach to guarantee a global solution of the flexibility index problem also for some non-convex problems. More recently, Li et al. [54] suggested a framework to calculate the flexibility index by means of an alternating direction matrix embedded in a Simulated Annealing algorithm. Additionally, Kachacha et al. [55] proposed to conduct Monte Carlo network simulations in the entire expected disturbance range while manipulating degrees of freedom. If sufficiently many operating points are tested, the shape of the feasible uncertainty space is identified. Furthermore, Zhao and Chen [56] proposed to explicitly calculate the shape of the feasible uncertainty space via cylindrical algebraic decomposition and quantifier elimination.

In the context of flexibility analysis of HENs, a distinction is made depending on the set of constraints which are included in the flexibility analysis. When only structural constraints (e.g. heat and mass balances) are considered, and no design constraints (e.g. heat transport equations of HEX), the term structural flexibility can be used. Marselle et al. [50] distinguished for example between a resilient network structure and a resilient network itself. In addition, Marselle et al. [50] suggested that a network structure is resilient if it remains feasible for the specified disturbance range independently of the HEX areas (i.e. HEX areas are not specified). A resilient network structure is, thus, the premise for a resilient network which remains feasible for the specified disturbance range for specified HEX areas [50]. This definition of structural resilience was later used by Li et al. [57] to describe structural flexibility of HENs.

In this thesis, a distinction is made between structural feasibility of a design and (general) feasibility of a design. Both can be assessed by solving the flexibility index problem. In the case of structural feasibility assessment, design constraints are discarded, and only structural constraints are considered, i.e. the heat transferred by HEXs is not limited by design characteristics. In the case of (general) feasibility assessment, design constraints are included, i.e. the heat transferred by HEXs is limited by design characteristics meaning that the installed surface area as well as the overall heat transfer coefficient of HEXs are considered. In contrast to the literature on the flexibility (or resilience) index, in this thesis the term (structural) flexibility is not used to describe the solution of the flexibility index problem. Instead the terms structural and general feasibility are suggested as the flexibility index provides information on the maximum disturbance range within which feasible operation can be achieved (see above). The term flexibility can however include other operational aspects, e.g. the capability to operate energy-efficiently or cost-efficiently at multiple operating points. In such a case, structural and general feasibility are the premise to be able to achieve flexibility.

2.4 Multi-Period Optimization

In multi-period optimization, an optimization model is solved considering multiple periods. This implies that the solution of a multi-period optimization problem may not be optimal for a single period among the considered periods, which is the decisive difference compared to a single-period optimization model. One example of a multi-period optimization problem is the design problem of a HEN operating during multiple periods. The solution of the multi-period HEN design problem indicates the design characteristics of the equipment (e.g. surface areas of HEXs) for a given HEN structure to achieve the optimal objective value over all considered periods. (see, e.g. [58]). The multi-period HEN design problem must not be mistaken for the superstructure-based multi-period HEN synthesis problem (see [41]) where also the structural layout of the HEN is derived.

In multi-period optimization, e.g. a multi-period HEN design problem, a sufficient number of sets of operating points need to be considered to guarantee feasibility and cost efficiency of the achieved solution (if the objective function is a cost function). However, with an increasing number of sets of operating points, the complexity of the problem increases. The computational capacity can be a limiting factor, especially for large-scale industrial HENs. To overcome these difficulties, different works in the literature deal with the reduction of the sets of operating points, e.g. by defining representative operating points (see, e.g. [59]) or by the identification of critical operating points [58, 60] (see Section 2.5) of a given structural design proposal. In comparison to representative operating points which should represent the entire operating period to achieve cost efficiency, the main idea of considering critical operating points is to ensure feasibility for the entire operating period. To ensure feasibility, critical operating points represent those variations (within a given uncertainty span) of the uncertain parameters which require the largest equipment size and are, thus, critical for design and operation of the HEN (see Section 2.5). This implies that the HEN itself must be structurally feasible and the feasibility may only be limited by design characteristics, i.e. HEX surface area and heat transfer coefficients (see Section 2.3).

The identified critical operating points can be utilized to find the necessary oversizing of HEXs in a given HEN structure. As mentioned previously, by including the identified critical points in the design problem, feasibility for the entire uncertainty span can be achieved. Additionally, representative operating points/scenarios may be identified, e.g. by screening of historical data, and included in the design problem to achieve a cost-efficient solution (cost-optimal for the representative operating points/scenarios and feasible for the set of critical points). To conclude, the HEN design problem subject to critical and representative operating points/scenarios can be expressed as the following multi-period MI(N)LP optimization problem:

$$
\begin{aligned}
&\min_{x,z,d} TAC = \sum_{s \in S} [w_s \cdot c_{operating,s}] + c_{investment} \cdot CRF \\
&\text{s.t.} \\
&\left.\begin{array}{l}
h_i(d,x,z,\Theta_{op}) = 0;\ i \in I \\
g_j(d,x,z,\Theta_{op}) \leq 0;\ j \in J \\
g_d(x,z,\Theta_{op}) - d \leq 0;\ d \in DV \\
d \geq 0 \\
x,z,d,\Theta_{op} \in \mathbb{R} \\
\Theta_L \leq \Theta_{op} \leq \Theta_U
\end{array}\right\} \quad op \in (S \cup CP).
\end{aligned}
\tag{2.11}
$$

In Problem 2.11, TAC represents the total annualized cost of the HEN design, which is described by the annual operating cost $c_{operating}$ in €/year (utility cost) of a number of defined representative operating points/scenarios $s \in S$ which are weighted with their normalized duration factor w_s (time period represented by operating point divided by entire time period), and the investment cost $c_{investment}$ in € (e.g. HEX investment cost) which are annualized with a given capital recovery factor CRF. The set of equality constraints is depicted by h_i with $i \in I$ (heat and mass balances) and the set of inequality constraints is represented by g_j with $j \in J$ (temperature and other operational restrictions). The set of design constraints g_d depends on the set of the non-negative design variables d with $d \in DV$. In h_i, g_j and g_d, x is the vector of the state variables, z corresponds to the control variables and the varying inlet conditions or uncertain parameters are depicted by Θ. Consequently, in order to find the optimal value for TAC (for the respective operating points), the degrees of freedom of the optimization problem are the non-negative design variables d with $d \in DV$ and the control variables (of the HEN) z. The set of constraints must be satisfied at all representative operating points/scenarios $s \in S$ and at all identified critical operating points $c \in CP$, i.e. for certain, previously identified, fixed combinations of values for the uncertain parameters. In Problem 2.11, the set of constraints must be satisfied at each operating point present in the union of the two sets S and CP: $op \in (S \cup CP)$. This way, a feasible and cost-efficient design is achieved.

2.5 Critical Point Analysis

To identify those variations (within a given uncertainty span) which require the largest equipment size, sensitivity analyses can be used if monotonic correlations between uncertain parameters and design variables exist [60]. One example is the correlation between the uncertain heat transfer coefficient and the surface area of a HEX – the maximum area of the HEX is obtained at the smallest value of the heat transfer coefficient within the uncertainty span [60]. However, it can be assumed that not many parameters follow these clear correlations and critical operating points can be determined following the procedure introduced by Pintarič and Kravanja in [58] which is based on the following idea:

> "The main idea is to identify points with the largest values of design variables at optimum objective function. This may be achieved by maximizing design variables one by one, while allowing uncertain parameters to obtain any value between the specified bounds, and simultaneously minimizing cost function." [58] (p. 1607)

This implies a max-min problem for each design variable $d \in DV$, i.e. maximizing the design variable of interest d_i while minimizing the cost function $C(x, z, d, \Theta)$, which is stated in Problem 2.12. Compared to the cost function in Problem 2.11 (TAC), in the cost function of Problem 2.12 ($C(x, z, d, \Theta)$) the operating cost of the representative operating points are not included [58]:

$$
\begin{aligned}
&\max_{\Theta} d_i = \min_{x,z,d} C(x, z, d, \Theta) = c_{operating} + c_{investment} \cdot CRF \\
&\text{s.t.} \\
&h_i(d, x, z, \Theta_{op}) = 0;\ i \in I \\
&g_j(d, x, z, \Theta_{op}) \leq 0;\ j \in J \\
&g_d(x, z, \Theta_{op}) = d;\ d \in DV \\
&d \geq 0 \\
&x, z, d, \Theta \in \mathbb{R} \\
&\Theta_L \leq \Theta \leq \Theta_U.
\end{aligned}
\tag{2.12}
$$

To solve the max-min problem, Pintarič and Kravanja [58] developed different formulations:

- The Karush-Kuhn-Tucker (KKT-)formulation;
- The two-level formulation; and
- The approximate one-level formulation.

By means of these formulations, possible candidates for critical points are identified. In a second step, a set covering algorithm is applied to the identified candidates to merge them into a final set of critical points. Both, the two-level and the approximate one-level formulation, approximate the solution of the KKT-formulation. Moreover, the approximate one-level formulation is dependent on a heuristically chosen large scalar (comparable to a Big-M parameter) and solutions can be very sensitive to this parameter. Additionally, if the system is convex all critical points are vertices of the uncertainty space. These critical vertices can be identified by solving Problem 2.11, excluding the representative operating points, sequentially at all vertices. Those vertices at which the maximum values for each design variable are obtained are critical. [58]

3

Results - Developed Approaches

As outlined in the introductory chapter, three papers are appended to this thesis. In each paper, one approach was suggested which advances a retrofitting problem by dividing it into sub-problems. All three approaches evaluate retrofit design proposals which have been defined beforehand. In this way, retrofit design methods can be applied to generate different design proposals with a reasonable level of effort (e.g. single-period, graphical approaches). The different design proposals are incorporated into a superstructure to be evaluated by one (or several) of the proposed approaches. Consequently, the superstructure represents all design proposals that are considered. The three different approaches are outlined in in the following three sections which are named similarly to the related paper appended to this thesis.

3.1 A Computational Tool for Guiding Retrofit Projects of Industrial Heat Recovery Systems Subject to Variation in Operating Conditions

In Paper I, a computational tool based on automated mathematical modelling of HENs is proposed which can be used to screen the previously defined design proposals. The tool allows for calculation of temperatures and heat loads in a HEN that is exposed to variations in inlet conditions and/or adjustment of operational settings; i.e. the computational analysis tool can be used to calculate the network response of a HEN (see Section 2.1). Evaluating the network response during screening processes is vital to gain information regarding performance and or cost of the different design proposals. The tool is intended as an alternative to detailed simulation models and/or iterative (trial-and-error) calculations (for evaluating the network response) which can be computationally burdensome, especially for large-scale problems. Furthermore, the tool includes a systematic method for defining complex network topologies. As a result, the complete set of equations necessary to describe the heat and mass balances of a given HEN can be generated automatically. Consequently, automated HEN modelling allows the network response of HENs of any size to be calculated automatically, with stream splitting and mixing, and with re-circulating streams and closed circulation loops. Furthermore, automated HEN modelling is of high interest for other advanced HEN analysis methodologies, e.g. for the calculation of the flexibility index (see Section 2.3).

The proposed analysis tool can be utilized to generate sensitivity tables to analyze the influence of varying operating data, adjusted operational parameters and design modifications on the network's response. These tables are generated by repeatedly calculating the network's response (i.e. temperatures and duties of HEXs) for defined variations in operating data but also adjustments of design characteristics (e.g. area of a new HEX) or operational settings (e.g. split ratio). The concept of HEN analysis based on sensitivity tables was introduced by Kotjabasakis and Linnhoff in [45]. In comparison to the manual derivation of the sensitivity tables introduced in [45], sensitivity tables can be generated automatically by means of the proposed analysis tool.

The proposed analysis tool enables the designer to conveniently assess the effect of manipulating operational parameters such as split ratios and bypass ratios. The main objective of such manipulation is to ensure operability (e.g. meet predefined operational targets) and to optimize savings (e.g. steam savings) for all (tested) operational data sets. A procedure for integrating the proposed analysis tool in retrofitting processes of HENs was proposed in Paper I and is outlined in Subsection 3.1.3. Additionally, the procedure was applied in the screening process of a retrofit design project on the HENs of the secondary heating system of a Kraft pulp mill and the results are presented in Paper I. Moreover, there is great potential for applying the computational analysis tool and the automated HEN modelling strategy in the approaches presented in Papers II and III. This will be explained in more details in the corresponding Sections 3.2 and 3.3. The necessary assumptions to apply the computational tool and the basis for the automated HEN modelling strategy are presented in Subsections 3.1.1 and 3.1.2.

3.1.1 Assumptions

As mentioned previously, the computational analysis tool allows calculation of the network response of an arbitrary HEN. It should be noted that when applying the P-NTU method, the set of equations that describes the HEXs present in the HEN is linear in the (unknown) network temperatures (compare Equations 2.5a and 2.5b). To apply the P-NTU method, the following assumptions are necessary:

- Heat capacity flow rate (CP-value) of each stream (and sub-stream resulting from splitting, mixing and switches) is constant and known;
- UA-value (overall heat transfer coefficient multiplied by the heat surface area) of each HEX is constant and known; and
- Type and flow arrangement of each HEX is known.

The assumption that the heat capacity flow rates of the streams are constant implies that the entire set of equations to model a HEN mathematically is linear in the network temperatures (compare Equations 2.4a, 2.4b, 2.5a, 2.5b and 2.7 to 2.9b). Consequently, a mathematical model for an arbitrary HEN which is based on the P-NTU method can be solved as a linear equation system to obtain the (unknown) network temperatures.

As the overall heat transfer coefficients (U-values) of the HEXs usually vary with temperatures and/or CP-values, assuming constant UA-values when variations in temperatures and flow rates are introduced introduces a simplification of the actual problem. To avoid this simplification, thermodynamic modelling and iterative calculations may be necessary. However, it is assumed that in early design stage screening, a certain degree of simplification is a valid trade-off between accuracy and computational expense. Therefore, temperature-dependencies of U-values are neglected. On the other side, there exist simple approaches (e.g. correction factors) to account for the dependency of the U-value if given CP-values differ from design values. In the proposed analysis tool, a correction factor which was introduced and studied by Persson and Berntsson in [15] has been implemented. This correction factor uses a simplified correlation between the heat transfer coefficient and the flow rate of a stream. Further details can be found in [15].

The assumptions made to achieve a linear HEN model imply certain limitations of the computational tool. These and other limitations are as follows:

- Temperature dependency of U- and CP-values are not considered (the correction factors included only consider dependency of U-values on varying CP-values);
- Phase-changing streams are not considered;
- The tool is limited to calculating the network's response to variations in network supply temperatures, heat capacity flow rates and U-values as well as adjustments of design characteristics (e.g. HEX area) and operational parameters such as HEX bypass ratios, split ratios and flow rates of utility streams (loads of utility exchangers); and
- The tool can be used for conducting sensitivity analyses on all input parameters; optimization algorithms to identify the optimal setting of operational parameters to a certain objective, e.g. minimize steam demand, are not incorporated.

3.1.2 Automated Heat Exchanger Network Modelling

To model a HEN, the network structure or topology needs to be described, i.e. the existence and the position of physical components described in Section 2.2. This can be challenging for large and complex networks due to the presence of a high number of HEXs, multiple streams splits, re-circulation of streams and closed circulation loops. A general methodology has been developed to model the topology in a straightforward way. In a first step, each stream of the HEN is numbered. To handle stream splits, re-circulation of streams and closed circulation loops, streams are numbered with respect to their CP-values and identities. This means that a stream in the modelling sense needs to have a constant CP-value and fixed identity. A stream split where one stream is split into two streams is, thus, counted as three individual streams. If the two split streams are mixed back together a fourth stream is counted. Figure 7 shows the classical grid representation of an example network. The streams are numbered according to the proposed numbering procedure. Furthermore, all (unknown) network temperatures with respect to equation 2.1 are marked.

For re-circulation of streams and closed circulation loops, switches are used which define the locations where the identity of streams changes (see Subsection 2.2.3). Consequently, with each switch a new stream is introduced. A specific example can be seen in Figure 7.

Besides stream numbering, a generalized way to refer to the location of a specific process-to-process HEX (P2P) or utility HEX (utility) is needed. Basically, this includes the (process) streams which are exchanging heat by means of the HEX as well as the location of the specific HEX on those streams. For this reason, a system to specify the position of the HEXs was developed which is based on the stream numbering. For each HEX, the hot and cold stream as well as the position of the HEX on these streams must be known.

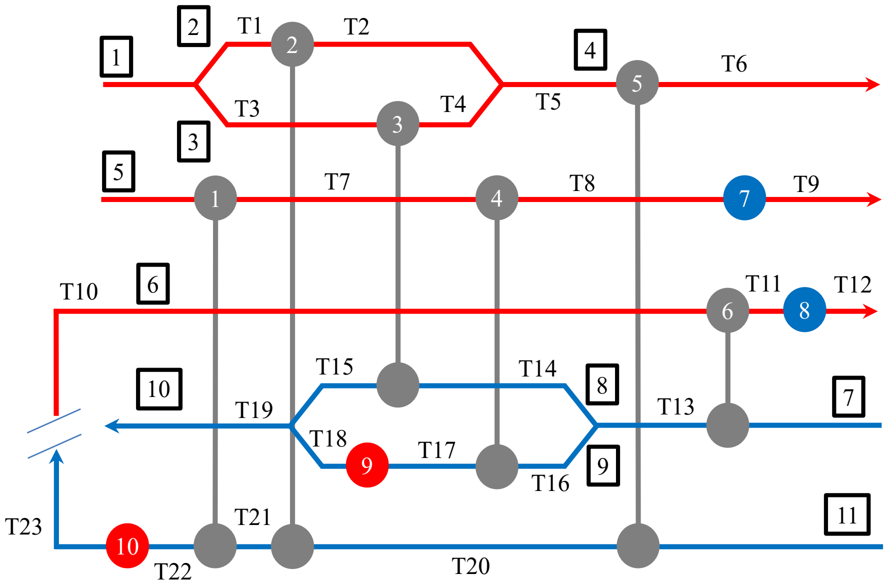


Figure 7: A second example heat exchanger network illustrating the stream numbering and (unknown) network temperatures.

For utility HEXs, a target temperature is specified in order to calculate the duty of each utility HEX (see Subsection 2.2.1). For the network depicted in Figure 7, the following location matrix for the HEXs can be derived (see Table 1).

Table 1: Exchanger location matrix of the example HEN for defining the position of all process-to-process (P2P) and utility exchangers and the target temperatures of streams with utility exchangers.

		Hot streams		Cold streams			Only for type “utility”
Ex-changer (HEX)	UA	Stream number	HEX number on stream	Stream number	HEX number on stream	Type (P2P or utility)	Target temperature (after exchanger)
1	UA1	5	1	11	2	P2P	
2	UA2	2	1	11	3	P2P	
3	UA3	3	1	8	1	P2P	
4	UA4	5	2	9	2	P2P	
5	UA5	4	1	11	4	P2P	
6	UA6	6	1	7	1	P2P	
7		5	3			utility	Ttarget,5
8		6	2			utility	Ttarget,6
9				9	1	utility	Ttarget,9
10				11	1	utility	Ttarget,11

In Table 1 and Figure 7, the position of the HEXs is determined by looking from left to right which in this case is the grid flow direction of the hot streams. In general, different ways are possible and can be implemented in the tool. A similar positioning system is used to describe the location of stream splits and mixing of streams. It is also based on the introduced stream numbering system. Table 2 presents the location matrix for the stream splits and mixes for the example network in Figure 7.

Table 2: Split/mix location matrix describing the position of all stream splits and mixes of the example network.

	Split streams			Mix streams		
Index	In	Out1	Out2	In1	In2	Out
1	1	2	3	2	3	4
2	7	8	9	8	9	10

To describe the location of switches, the ingoing and the outgoing streams must be specified, and a similar location matrix can be derived. Table 3 shows the location matrix for switches of the example network in Figure 7.

Table 3: Switch location matrix describing the position of all switches of the example network.

	Switches	
Index	In	Out
1	11	6

Based on the exchanger location matrix, the split/mix location matrix and the switch location matrix, the vector of the (unknown) network temperatures, T, can be sorted in a data structure called temperature matrix. In this data structure, the (unknown) network temperatures are allocated to the process streams. The allocation process is automated in the proposed analysis tool. The basis for this automatization is Equation 2.1. In this context, one element of T (unknown network temperatures, see Figure 7) is allocated to a stream if the stream is connected to a HEX (P2P or utility). Furthermore, one element of T is allocated to each stream resulting from a split, mix or switch. This way, all (unknown) network temperatures can be allocated to the different streams. Therefore, one dimension in the temperature matrix represents the streams present in the HEN.

The temperature matrix for the example network is shown in Table 4. As mentioned previously, the rows of the temperature matrix represent the different process streams (row number equivalent to stream number in Figure 7), while the number of columns represent the number of (unknown) network temperatures of the corresponding process stream. As the number of (unknown) network temperatures may be different for the individual process streams, a data structure which accounts for this must be used (e.g. “Cell Array” in MATLAB or “List of Lists” in PYTHON).

The temperature matrix is the basis for the automated HEN modelling strategy as it allows for allocating the elements of T (unknown network temperatures, see Figure 7) to specific HEXs (P2P and utility), stream splits, mixing points and switches. The allocation of the (unknown) network temperatures is vital to be able to derive the set of energy

Table 4: Temperature matrix to allocate (unknown) network temperatures of the example network to specific exchangers (process-to-process and utility), stream splits, mixing points and switches.

Stream	(Unknown) network temperatures				
1	$T_{in,1}$				
2	$T1$	$T2$			
3	$T3$	$T4$			
4	$T5$	$T6$			
5	$T_{in,5}$	$T7$	$T8$	$T9$	
6	$T10$	$T11$	$T12$		
7	$T13$	$T_{in,7}$			
8	$T15$	$T14$			
9	$T18$	$T17$	$T16$		
10	$T19$				
11	$T23$	$T22$	$T21$	$T20$	$T_{in,11}$

and mass balances presented in Section 2.2 automatically with the correct elements of T. This is illustrated by means of HEX 1 of the example network shown in Figure 7:

> Based on the exchanger location matrix (Table 1), the two process streams which are connected by HEX 1 are hot stream 5 and cold stream 11. Additionally, the position of HEX 1 on these two streams is specified in the exchanger location matrix. For hot stream 5, HEX 1 is the first exchanger (counting from left to right) on this stream. Thus, the hot stream inlet temperature of HEX 1 is the inlet temperature of stream 5, $T_{in,5}$, while the hot stream outlet temperature of HEX 1 is $T7$ (elements 1 and 2 for stream 5 in the temperature matrix, Table 4). For cold stream 11, HEX 1 is the second exchanger on this stream. Thus, the cold stream outlet temperature of HEX 1 is $T22$ while the cold stream inlet temperature of HEX 1 is $T21$ (elements 2 and 3 for stream 11 in the temperature matrix, Table 4). Consequently, the unique elements of T which are present in Equations 2.5a and 2.5b for HEX 1 can be identified.

As the example for HEX 1 shows, by means of the exchanger location matrix and the temperature matrix, specific elements of T are allocated to each HEX. Similar allocations can be achieved by means of the split/mix or the switch location matrix to allocate (unknown) network temperatures to the corresponding split, mix or switch. Consequently, the set of equations for an arbitrary HEN (see Section 2.2) can be derived automatically. It should be noted that automated HEN modelling is also of high interest for other advanced HEN analysis methodologies, e.g. feasibility analysis or critical point analysis and examples for possible applications can be found in Sections 3.2 and 3.3.

3.1.3 Proposed Procedure for Integrating the Computational Analysis Tool in a HEN Retrofit Project

In Paper I, a procedure is proposed to utilize the computational analysis tool to screen HEN retrofit measures as well as HEN greenfield design proposals. It should be noted that the computational analysis tool is not bound to any specific objective when evaluating different design proposals (e.g. cost efficiency and/or energy efficiency). This allows a certain degree of flexibility since the designer can adjust the objective during the design process. The procedure for utilizing the computational analysis tool in a HEN retrofitting project is described below and visualized in Figure 8:

1. Definition of retrofit design proposals (e.g. by means of graphical retrofitting methodologies) and incorporation of proposals in a superstructure;
2. Identification of operational data sets representing different combinations of inlet conditions, i.e. operating points, during the operating period of the HEN – inlet conditions are supply temperatures, heat capacity flow rates and (film) heat transfer coefficients;
3. Generation of mathematical models of the different design proposals by means of the automated HEN modelling strategy (see Subsection 3.1.2) and further:
    - Identification of operational parameters which can be adjusted during operation of the HEN – operational parameters are split ratios and bypass ratios of HEXs;
    - Definition of operational constraints which define the operability of the HEN, e.g. stream target temperatures;
4. Comparison of retrofit design proposals by means of the computational analysis tool following the two steps below:
    - Evaluation of the network's response of each retrofit design proposal for the identified operational data sets;
    - Adjustment of operational parameters (e.g. split ratios) and consideration of (minor) design changes to ensure operability and optimize with respect to a defined objective (e.g. cost efficiency and/or energy efficiency) throughout the entire operating period by means of sensitivity analyses; and
5. Identification of the design alternative(s) which fulfills a defined objective (e.g. most cost-efficient and/or most energy-efficient).

It should be noted that the final step of the procedure is not illustrated in Figure 8. As mentioned in the beginning of Section 3.1, the proposed computational analysis tool was utilized to screen different retrofit design proposals of a subsystem of the secondary heating system of a Swedish Kraft-Pulp mill. A Pinch analysis conducted prior to the study revealed that there is potential for increased heat recovery in the mill's secondary heating system. Using the results of the Pinch analysis, one subsystem within the secondary heating system was identified in which 36.5 % of the total Pinch rule violations identified occur. Four retrofit design proposals were developed using graphical Pinch analysis considerations in order to reduce the identified Pinch rule violations. These retrofit proposals were derived based on average values representing spring operating conditions at the mill. Since the mill in question operates year-round, in a next step operational data sets representing the other annual seasons (i.e. summer, autumn and winter) were collected in cooperation with mill experts. Furthermore, operational constraints were de-

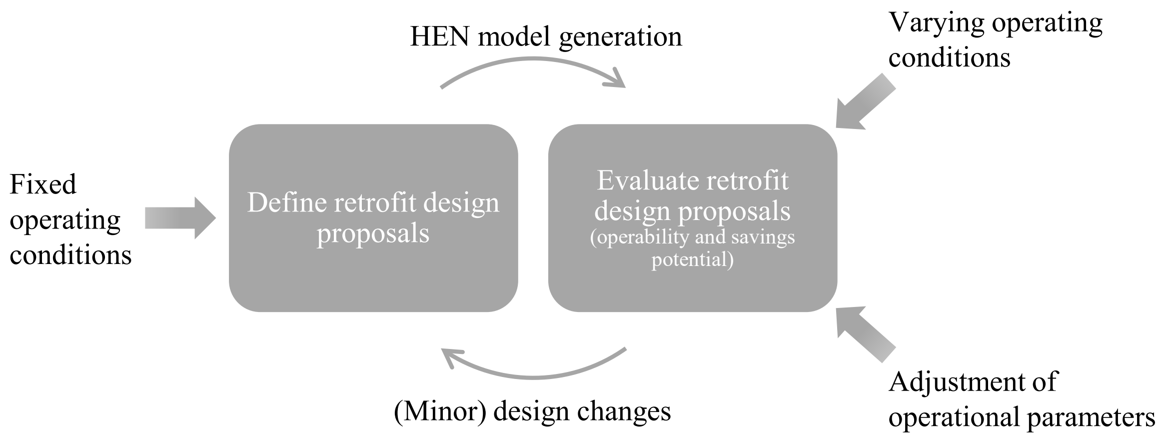


Figure 8: Proposed procedure for applying the computational analysis tool to a heat exchanger network retrofit project.

fined and operational parameters which can be adjusted during operating were identified by consulting mill experts. The computational tool was then utilized to evaluate the different design proposals when operating conditions vary. The main focus of the evaluation was to ensure operability and to maximize energy efficiency during all operating periods. For this reason, adjustment of operational parameters was considered in order to decrease the demand for external utility (e.g. steam). Sensitivity analyses based on sensitivity tables were performed to identify the impact of changing operational settings on the utility demand as well as operational target values. In a final step, the achieved utility savings of the different retrofit proposals were compared for the different seasons. The results indicated that one proposal is promising as a result of the moderate level of investment cost (based on HEX area demand). Furthermore, for two of the four operational data sets, this proposal achieves the highest energy cost savings (and the second highest in the remaining two periods).

3.2 Combined Flexibility and Energy Analysis for Retrofit Measures of Heat Exchanger Networks

Paper II proposes a method to combine flexibility and energy analysis. By means of combined flexibility and energy analysis, the previously defined design proposals (see first paragraph of Chapter 3) are evaluated to identify those proposals which can operate energy-efficiently for a predefined range of operating conditions. For performing this analysis, a systematic approach was developed. The proposed approach is outlined in the following subsections. An illustrative example is presented in Paper II. In Paper II, the term flexibility analysis refers to the calculation of the flexibility index (see Section 2.3). In accordance with Section 2.3, the flexibility index can be used to assess the structural and general feasibility of a HEN. Therefore, the term feasibility assessment is hereafter used to refer to the calculation of the flexibility index. However, to avoid confusion with Paper II the term "combined flexibility and energy analysis" is maintained.

3.2.1 Feasibility Assessment

In the first step of combined flexibility and energy analysis, the feasibility of the design proposals is assessed (by means of the flexibility index, see Section 2.3). With feasibility assessment, it can be verified that HEN operation remains feasible within a certain predefined range of disturbances. This applies for structural and general feasibility (see Section 2.3). While proposals which are structurally infeasible can be excluded from further analysis, design characteristics such as HEX surface areas of structurally feasible proposals may be adjusted to achieve general feasibility (if general feasibility is not achieved with the original design characteristics). In Paper II, it is proposed to adjust the design characteristics in a trial-and-error manner until general feasibility is achieved. In order to perform the structural and the general feasibility assessment, mathematical modelling of the HEN is required (see Section 2.3). This can be cumbersome, especially if many design proposals with numerous (adjustable) design characteristics need to be evaluated. To avoid manual mathematical HEN modelling, the automated HEN modelling strategy developed in Paper I (see Subsection 3.1.2) can be applied.

The flexibility index can be calculated by means of the one of the approaches presented in Section 2.3, namely:

- Active set approach (see [53]);
- Alternating direction matrix (see [54]);
- Cylindrical algebraic decomposition and quantifier elimination (see [56]); and
- Monte Carlo network simulations (see [55]).

However, all approaches for calculating the flexibility index have drawbacks. The active set approach may result in impractically large problem formulations as industrial applications are often complex. The alternating direction matrix approach relies on the simulated annealing algorithm, which means that the global solution may not be found in a reasonable period of time. Applying cylindrical decomposition to industrial applications (which typically involve more than four HEXs and uncertain parameters) requires excessive computational capacity, which may not be available. The same applies for Monte Carlo network simulations, especially if the number of uncertain parameters is high and/or the HEN is structurally complex. Although all listed methodologies for (structural) feasibility assessment have known drawbacks, it is assumed in this thesis that feasibility assessment of the HENs in question is possible. The active set approach was considered to be most appropriate because it is the only deterministic approach among those listed (excluding cylindrical decomposition). This is further discussed in Chapter 4.

3.2.2 Energy Performance Analysis

From the results obtained during feasibility assessment, no conclusions can be drawn regarding the energy performance of the HEN when the disturbances occur. The idea of combined flexibility and energy analysis is to extend feasibility assessment, which provides information on the level of feasibility (see Subsection 3.2.1), by providing additional information on the energy performance of a HEN when exposed to variations. Prior to any advanced analysis, it can be concluded that certain variations have certain consequences on the energy performance, e.g. if all inlet temperatures vary in a negative direction, the heating requirements will increase [50]. However, such statements may only provide vague information on the performance of a HEN as the following examples illustrate:

1. If the maximum energy recovery (MER) targets of a stream data set result in high utility demand, a HEN achieving these targets performs optimally from an energy perspective although the utility demand is high in absolute numbers; and
2. If a HEN's utility demand is higher than the utility MER targets, this network does not perform at the optimal energy level although the utility demand may be low in absolute numbers.

Consequently, it is necessary to define assessment criteria for the energy performance of a HEN exposed to variations. In the literature there is a lack of published methods for assessing the energy performance of a HEN exposed to variations. Attempts were made by Marselle et al. [50] and Saboo et al. [51]. According to Marselle et al. [50], a HEN (with fixed heat exchanger areas) is resilient if it can achieve MER for the specified disturbance range. MER for the specified disturbance range is explicitly defined as "that for a specific ΔT_{min} and any inlet condition within the disturbance range, maximum energy recovery, as determined by the assumed perturbed inlet conditions, can be achieved" [50] (p. 261). In the formulation of the resilience index, Saboo et al. [51] introduced an MER constraint (which can be relaxed) to define feasible operation if the utility consumption at any point within the disturbance range does not exceed the MER-conditions specified for the initial design point. However, this constraint does not allow a fair comparison since, due to the variations in the stream data, the utility MER targets change for every operating point, as indicated by Marselle et al. [50]. Therefore, a novel assessment criterion is proposed in Paper II for analyzing the energy performance of a HEN exposed to variations by energy performance ratios (EPR). The ratios between the "updated" utility MER targets ($Q_{MER,i}$) for each possible set of variations (i) (which can be interpreted as individual stream data sets) and the actual utility demands ($Q_{utility,i}$) of the HEN for each possible set of variations (i) are proposed to achieve energy performance ratios (EPR_i). These EPRs enable fair comparison of all sets of variations (I):

$$EPR_i = \frac{Q_{MER,i}}{Q_{utility,i}} \; \forall \; i \in I. \tag{3.1}$$

The calculation of EPRs implies two essential problems:

1. For each possible set of variations, the MER targets need to be calculated. Since there are infinitely many sets of variations in a defined range of disturbances this requires calculations of an infinite number of MER targets; and
2. The network response needs to be calculated for each possible set of variations to obtain the actual utility demand of the HEN considered which consequently results in an infinite number of problems.

Thus, it is necessary to explicitly define operating points to perform the above-mentioned calculations which implies that the problem size depends on the number of chosen operating points. Different strategies are possible to deal with this issue, and in Paper II the most extreme operating points (maximum disturbance) were selected. For the second problem mentioned above, the computational analysis tool developed in Paper I (see Section 3.1) can be used. However, the large number of degrees of freedom or control variables of a HEN can be problematic. For example, bypass ratios, split ratios, etc. may be manipulated to achieve the optimal utility consumption for each unique set of variations. Thus, trial and error manipulation, sensitivity analyses and/or optimization of these control variables is necessary. In the following subsection, a procedure is proposed for integrating the combined flexibility and energy analysis in a HEN retrofit project.

3.2.3 Proposed Procedure for Integrating Combined Flexibility and Energy Analysis in a HEN Retrofit Project

1. Definition of different retrofit design proposals:
   Different retrofit design proposals can be defined using single-period retrofit methodologies and are incorporated into a superstructure (see first paragraph of Chapter 3).
2. Feasibility assessment and identification of network modifications to resolve bottlenecks:
   The feasibility assessment can be divided into a structural and a general feasibility assessment. If a proposal is identified to be structurally infeasible, it can be excluded from further analysis. For general feasibility assessment, a formulation for the flexibility index problem including HEX design characteristics (see Section 2.3) is required. If the flexibility index problem initialized with the installed/preliminary design characteristics results in a value for the flexibility index which is ≥ 1, the designer can proceed directly to the energy analysis part (see step 3). If the flexibility index is smaller than 1, design modifications must be considered to increase the flexibility index. In the illustrative example of Paper II, the flexibility index was increased by increasing heat transfer in the heat exchangers which was modelled by increasing UA-values (in a trial-and-error manner). In practice, increased UA-values are equivalent to either increase of area or heat transfer enhancement.
3. Analysis of energy performance:
   This involves the calculation of MER targets and of the utility demand as well as the calculation of the above defined EPRs (see Equation 3.1) for each point of interest. As outlined, the computational analysis tool developed in Paper I can be utilized to calculate the denominator of the EPRs (see Equation 3.1). From an energy perspective, high values of the EPRs are desirable since they imply an energy performance that is near to optimum. Design modifications may be considered if EPR values are low (i.e. not satisfactory).
4. Evaluation of combined flexibility and energy analysis:
   The results provided by the combined flexibility and energy analysis enables the different proposals to be compared, e.g. by means of rigorous cost calculations.

The above described procedure is illustrated in Figure 9 in which the interconnections between the different steps are highlighted. The final evaluation step is not included in Figure 9.

As mentioned previously, the proposed procedure for integrating combined flexibility and energy analysis is illustrated by means of a HEN example in Paper II. In this example, two retrofit design proposals of a HEN were compared by means of the proposed combined flexibility and energy analysis. The analysis revealed that both proposals are structurally feasible. To achieve (general) feasibility, UA-values of HEXs were increased in a trial-and-error manner. It was identified that significantly different increases in UA-values (in

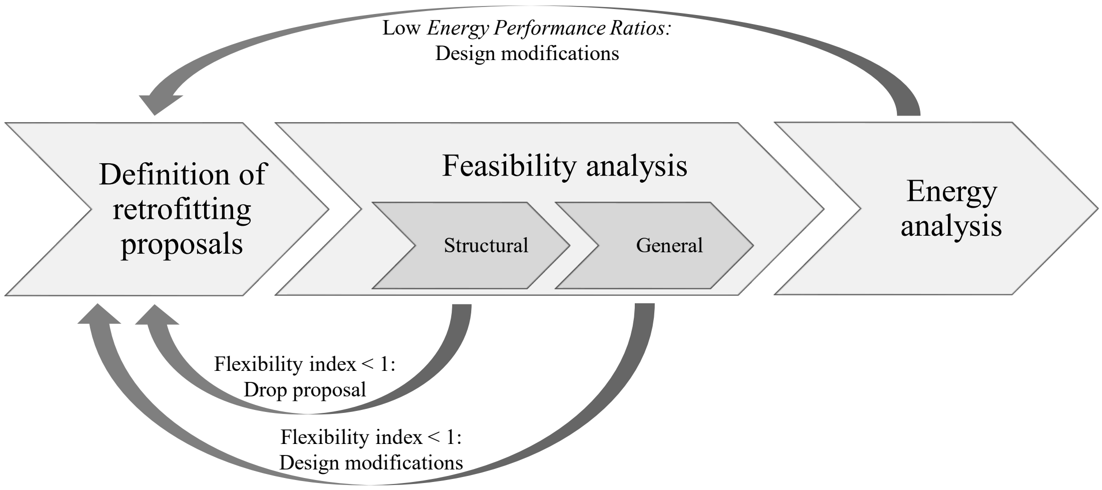


Figure 9: Proposed procedure for integrating combined flexibility and energy analysis in a HEN retrofit project.

absolute numbers) were necessary to achieve (general) feasibility. By means of the EPRs for the most extreme operating points (maximum disturbance), the energy performance of the two retrofit proposals was compared. The results revealed the difference in potential of the two retrofit proposals to increase energy efficiency. Additionally, the obtained results revealed further investment options which allow the designer to balance the trade-off between investment cost and operating cost prior to their quantification via rigorous cost calculations (i.e. the impact of different investment options on the energy efficiency could be quantified using the EPRs).

3.3 A Framework for Flexible and Cost-Efficient Retrofit Measures of Heat Exchanger Networks

In Paper III, a framework was developed which divides the retrofitting process into five sub-steps. In the title of Paper III, the term *flexible* was used to refer to retrofit measures which achieve general feasibility (see Section 2.3). In contrast to the title, the terms structural and general feasibility were used in Paper III to refer to the calculation of the flexibility index. The framework was inspired by the combined flexibility and energy analysis presented in Paper II (see Section 3.2). The idea was to combine feasibility assessment with multi-period optimization to derive design characteristics for the previously defined design proposals (see first paragraph of Chapter 3) which are feasible and cost-efficient at multiple operating points. The framework is shown in Figure 10 and the five sub-steps are outlined hereafter. A short description of the framework and a comparison with the combined flexibility and energy analysis presented in Paper II (see Section 3.2) is also presented.

After the incorporation of the design proposals in a superstructure, the design proposals which are structurally infeasible are discarded by means of structural feasibility assessment (see Section 2.3). Consequently, this structural feasibility assessment is performed in a similar way to the structural feasibility assessment proposed in Paper II (see Subsection

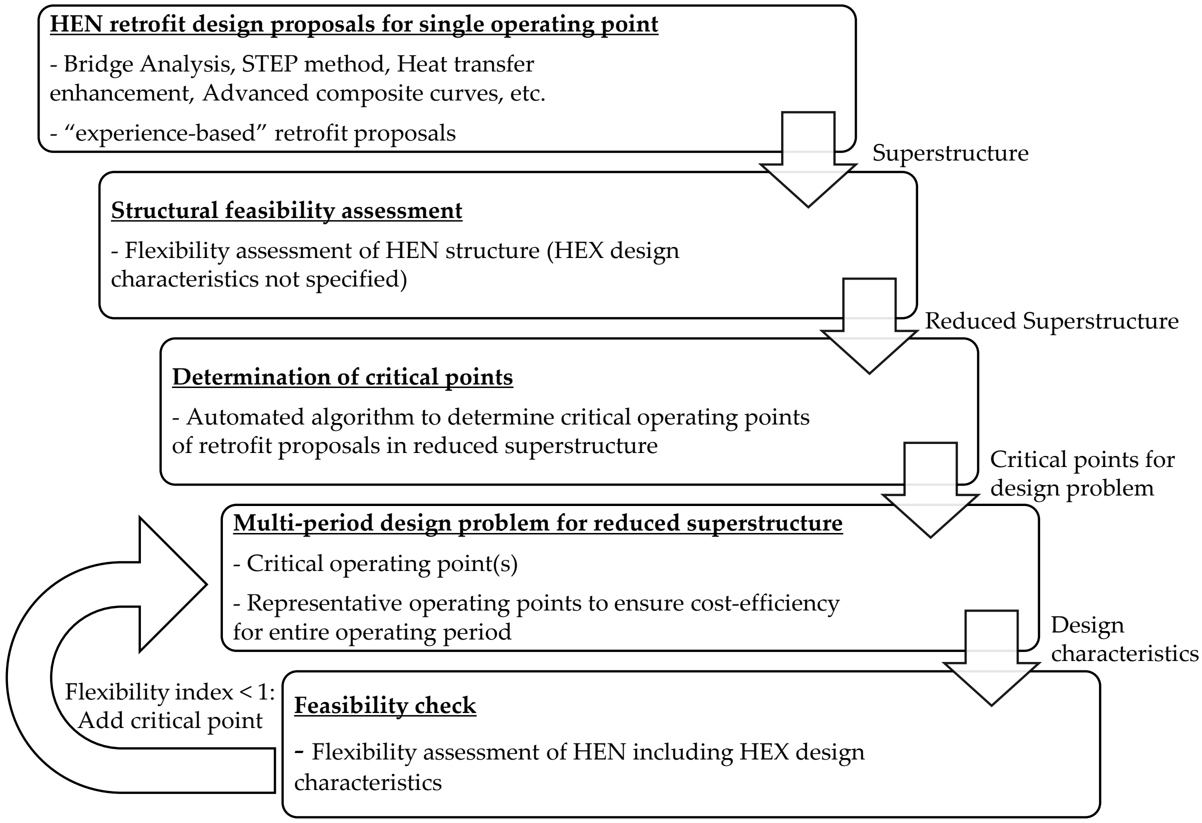


Figure 10: Retrofitting framework to achieve feasible and cost-efficient retrofit measures of heat exchanger networks (HENs).

3.2.1). However, in contrast to the trial-and-error adjustment of UA-values to achieve general feasibility proposed in Paper II (see Subsection 3.2.1), the framework presented in Paper III solves the multi-period HEN design problem (see Section 2.4) including critical and representative operating points. As outlined in Section 2.4, by means of critical points, feasibility of the design characteristics can be ensured for the entire uncertainty span while at the same time avoiding sub-optimal solutions due to unnecessary oversizing of equipment. Additionally, cost efficiency for the entire operating period is ensured by considering representative operating points besides the identified critical points (see Section 2.4). In addition to the multi-period HEN design problem, a final feasibility check is suggested to ensure that all critical points have been identified (i.e. the set of critical points is complete); otherwise, the new critical point, which is identified during this check, is added to the set of critical point(s) and the design problem is solved again.

Comparing the approaches presented in Paper II and Paper III, instead of solving the flexibility index problem multiple times with different UA-values (proposed in Paper II, Section 3.2), in Paper III it was proposed to solve the multi-period HEN design problem followed by a final (general) feasibility assessment. Furthermore, instead of an energy performance analysis for selected operating points to compare different feasible designs as proposed in Paper II (see Subsection 3.2.2), the multi-period HEN design problem (utilized in Paper III) yields the most cost-efficient design (which is also feasible) based on the provided design proposals.

3.3.1 HEN Retrofit Design Proposals for Single Operating Point — Generation of Superstructure

In this approach, and similarly to the two approaches presented in Papers I and II, design proposals are defined using single-period and well-proven retrofit design methodologies. The resulting design proposals are thereafter compiled in a superstructure which includes all design proposals that are considered.

3.3.2 Structural Feasibility Assessment — Reduction of Superstructure

In the next step, similarly to the approach presented in Paper II, the structural feasibility of the identified design proposals is analyzed by means of structural feasibility assessment. As outlined in Section 2.3, this can be done by calculating the flexibility index discarding all design constraints and considering only structural constraints. In Section 2.3 and Subsection 3.2.1, the different approaches to calculate the flexibility index are presented briefly. The drawbacks of the different approaches for calculating the flexibility index are discussed in Subsection 3.2.1. To reduce the probability of erroneous results, several of the proposed methods may be applied and the results be compared. If design proposals can be identified that are structurally infeasible for at least some operating points within the uncertainty span (i.e. flexibility index smaller than 1), these design proposals are excluded from further analysis as proposed in Paper II, yielding a reduced superstructure.

3.3.3 Determination of Critical Points

In the next step, critical operating points for each design proposal are identified using the different strategies for the identification of candidates for critical points and the set covering algorithm introduced by Pintarič and Kravanja [58] (see Section 2.5). Although Problems 2.11 and 2.12 were originally derived for HEN synthesis problems, they are structurally similar for HEN retrofitting problems. It should be noted that besides the investment cost of new HEXs, investment in existing equipment can also be considered, e.g. heat transfer enhancement or an increase of the area of existing HEXs, as well as structural changes, such as resequencing and repiping of existing HEXs.

It is worth mentioning that for the critical point analysis, each design proposal (which is present in the reduced superstructure) is considered individually, i.e. for each design proposal this step yields an individual set of critical points. To allow a fast evaluation of the different design proposals, the different strategies for the identification of candidates for critical points and the set covering algorithm proposed in [58] were automated in order to be applicable to a superstructure-based approach and industrial applications (see Supplementary Material of Paper III). Further automatization is possible, e.g. by utilizing the automated HEN modelling strategy presented in Paper I.

3.3.4 Multi-Period Design Problem for Reduced Superstructure

With all critical points obtained, the multi-period HEN design problem for the reduced superstructure and the representative operating points can be formulated. This problem is very similar to Problem 2.11, with the exception that each design proposal $p \in P$ may include a not generalizable number of individual equality constraints $i \in I_p$, inequality constraints $j \in J_p$, and design constraints/variables $d \in DV_p$ as well as an individual set of critical points $c \in CP_p$, which results in an individual set of operating points $op_p \in (S \cup CP_p)$ for which the set of constraints of the respective design proposal must be satisfied. Problem 2.11 can therefore be reformulated as follows:

$$\begin{aligned}
&\min_{x,z,d} TAC = \sum_{p \in P} y_p \cdot \sum_{s \in S} [w_s \cdot c_{operating,s,p}] + c_{investment,p} \cdot CRF \\
&\text{s.t.} \\
&\sum_{p \in P} y_p = 1 \\
&y_p \in 0, 1; \;\; p \in P \\
&\left.\begin{aligned}
&y_p \cdot h_i(d, x, z, \Theta_{op,p}) = 0; \;\; i \in I_p \\
&y_p \cdot g_j(d, x, z, \Theta_{op,p}) \leq 0; \;\; j \in J_p \\
&y_p \cdot [g_d(x, z, \Theta_{op,p}) - (d_{existing} + d)] \leq 0; \;\; d \in DV_p \\
&d \geq 0 \\
&x, z, d, \Theta_{op,p} \in \mathbb{R} \\
&\Theta_L \leq \Theta_{op,p} \leq \Theta_U
\end{aligned}\right\} \; op_p \in (S \cup CP_p).
\end{aligned} \tag{3.2}$$

In Problem 3.2, the set of individual design proposals of the reduced superstructure is represented by $p \in P$. Each design proposal is expressed via a binary variable y_p and one and only one of these binary variables is forced to be 1, which will be the design proposal, which performs most cost-efficiently at the representative operating points (and remains feasible at the corresponding critical operating points). As Problem 3.2 is to a large extend based on the equations present in an ordinary mathematical HEN model ($h_i(d, x, z, \Theta_{op,p}) = 0, \; i \in I_p$ and $g_j(d, x, z, \Theta_{op,p}) \leq 0, \; j \in J_p$ are likely to represent large parts of the problem), an adaption of the automated HEN modelling strategy presented in Paper I (see Subsection 3.1.2) to automatically derive Problem 3.2 for any given HEN case study allows further automatization and decreases the probability of erroneous modelling.

Instead of solving Problem 3.2 simultaneously, it may also be solved proposal-wise, setting one y_p to 1 and eventually comparing the TAC of all proposals to identify the most cost-efficient design proposal in the reduced superstructure. In this context, it should be noted that all costs that can be associated with the respective retrofit design proposal must be included in the respective cost functions $c_{operating,p}$ and $c_{investment,p}$. This is especially important for retrofitting projects of industrial HENs, which are often very interconnected, and which may cause increased cost in other operational units. It should be noted that in comparison to the traditional superstructure-based HEN synthesis problem (compare e.g. [25] or [41]) it is not necessary to define generic cost functions. In the proposed framework, the number of proposals is limited which allows to specifically define cost functions for each design modification considered.

3.3.5 Feasibility Check

In a final step, the (general) feasibility is checked by means of the methodologies presented in Section 2.3 and discussed in Subsection 3.2.1. This step is necessary to ensure that all critical points have been identified (i.e. the set of critical points is complete). As outlined in Section 2.3, the previously derived HEX design characteristics are included, i.e. design constraints and solutions obtained by solving the multi-period design problem. Since including design characteristics is likely to increase the complexity of the problem, solutions obtained by the methodologies listed in Subsection 3.2.1 should be analyzed with great care. Furthermore, it is advisable to compare the achieved results of different methodologies to reduce the probability of failures. If feasibility for the respective design cannot be guaranteed, the result of the feasibility check can provide useful insights. Besides the flexibility index, the feasibility check provides a point in the space of the uncertain parameters, which limits the flexibility index. The vector between this point and the average operating point (see Figure 6) can be used to generate additional candidates of critical points, which can be added to the multi-period design problem. If the newly generated design is feasible, the set of critical points has been successfully identified; otherwise, the new limit for the flexibility index is analyzed, and the step is repeated until a feasible design is obtained.

3.3.6 Illustrative Example

In Paper III, the proposed approach is illustrated by means of a four-stream HEN example (six HEXs) adapted from [42]. The proposed framework was utilized to compare different retrofit design proposals. Initially, five different design proposals were considered which were derived using graphical retrofitting methodologies. However, one design proposal was identified to be structurally infeasible by means of structural feasibility assessment and was discarded from further analysis. For the remaining proposals, the full set of critical points was obtained by means of the methodologies presented by Pintarič and Kravanja [58]. However, some modifications to the methodologies were necessary which are discussed in Appendix A of Paper III. In addition to the critical points, representative operating periods were defined in order to achieve cost efficiency for the entire operating period. The multi-period HEN design problem (Problem 3.2) was solved proposal-wise and the final feasibility check revealed that the achieved design characteristics were feasible for the expected variations in operating conditions. Additionally, the achieved TAC values were discussed to explain the impact of different assumptions which were made regarding the used data for investment and operating costs.

4
Discussion

In each of the three approaches for retrofitting HENs subject to variations in operating conditions, which have been outlined in this thesis and the appending papers, the retrofitting process is divided into several sub-steps. In the approaches outlined in Papers II and III (Sections 3.2 and 3.3), the flexibility index problem is solved to determine the structural feasibility as well as the (general) feasibility of different HEN designs (further information regarding structural and general feasibility is included in Section 2.3). In the context of feasibility analysis for HENs, the active set approach formulated by Grossmann and Floudas [53] is commonly applied since the methodology is deterministic. This is crucial because in comparison to alternative non-deterministic methodologies (see e.g. [54, 55]), with a deterministic methodology it is possible to provide proof that a found solution is the global solution. However, non-linearities due to complexities such as re-circulation, closed circulation loops but also multiple stream splits, inevitably lead to difficulties in finding feasible solutions with deterministic methodologies. In particular, if (deterministic) global optimization frameworks are applied, tight bounds on variables are crucial for the framework to converge and provide the global solution (which is only valid within the defined bounds).

Additionally, the active set approach for calculating the flexibility index is based on determining a priori the number of active inequality constraints at the solution by following the Haar condition (number of active inequality constraints is equal to number of control variables plus 1, see [53]). In this context, an inequality constraint becomes active when it reaches its bound (e.g. $5 + x \leq 8$ is active for $x = 3$) However, when modifying the operational inequality constraints of HEXs (see Equations 2.4a and 2.4b) to ensure that these constraints are not independent of the HEX duty (see Subsection 2.2.1), such a constraint would become active if the exchanger is bypassed, i.e. the duty of the HEX becomes 0. To avoid this, further work is necessary.

In the context of uncertain parameters which are input information for feasibility assessment but also for the determination of critical operating points, hidden or not obvious correlations between different uncertain parameters are important to identify prior to the analysis. In this thesis and the examples in Paper II and Paper III, it was assumed that no correlations exist between the uncertain parameters. However, as the example in Paper I illustrates, correlations between uncertain parameters are commonly present in industry (e.g. there is a common trend that all temperatures are at their lowest value during winter times, see Table 6 in Paper I). Additionally, different streams in industrial heat recovery systems may result from the same unit process which means that their flow rates are likely to follow the same trends depending, e.g. on the production rate of this unit process. It can be expected that in some cases these correlations influence the flexibility index and the critical point analysis. One example is that the feasibility could be limited by means of a combination of deviations (of the uncertain parameters) which represents a physically impossible operating point. Consequently, ignoring correlations can lead to underestimated feasibility and oversized equipment. An example for how correlations can influence the result of the flexibility index problem is discussed in Chapter 6.

All proposed approaches presented in this thesis depend on proposals for structural changes in advance to their application. With increasing structural complexity of the respective case study, graphical or graphical based design approaches can be advantageous due to their inherent suitability for user interaction. It should be noted that utilizing these single-period methodologies creates the risk that none of the derived retrofit design proposals is structurally feasible for the entire operating period as the feasibility assessment is done after the proposal generation. However, feasibility assessment provides an indication of why a design proposal is not feasible (see, e.g. "Final Feasibility Check" of Paper III, Section 3.3.5). Consequently, the definition of structurally feasible design proposals should be possible with some degree of iteration. Nevertheless, the generation of design proposals beforehand is one reason why global optimality of the final solution with respect to the retrofitting problem can never be guaranteed as the superstructure is limited to the provided design proposals. However, the main driver for industrial retrofitting projects is usually to achieve some although not necessarily the most optimal improvement compared to the current situation which allows sub-optimal solutions.

As mentioned in the introductory chapter, the complexity of industrial applications has many different degrees. An important one is the reliability, availability and other quality concerns of data. In particular, the importance of data must be highlighted for the generation of the structural proposals by means of single-period methodologies but also for the analysis steps which are proposed in the different approaches.

To achieve feasible and cost-efficient/energy-efficient design characteristics for structurally feasible design proposals, the three approaches outlined in this thesis utilize different strategies (compare Figure 3):

- Increase of UA-values (and adjustment of operational settings) via sensitivity analyses (Paper I);
- Trial-and-error increase of UA-values (Paper II); and
- Critical point analysis and multi-period optimization (Paper III).

In general, one can assume a correlation between the size of a HEN and the design possibilities to achieve (general) feasibility for structural feasible proposals (the larger the network, the more design possibilities). This results in high combinatorial complexity. In the case of manual approaches such as trial-and-error approaches or sensitivity analyses, finding all possible combinations of design characteristics which are feasible in order to identify the optimum combination can be cumbersome. Consequently, automatized approaches based on optimization are promising. On the other hand, optimization requires defining a specific objective function (which can be optimized) while the objective of manual approaches can be more vague and can easily be modified during the solution process. By means of this, the designer takes an active part in the design process which can be beneficial to identify trade-offs. Additionally, for typical industrial heat exchanger networks, significant computational power may be necessary to obtain a solution via optimization approaches. In conclusion, the selection of the approach is highly dependent on the overall (retrofitting) problem and the preferences of the designer. It seems, however, advisable to rely on more manual approaches for problems which are smaller in size but characterized by complex structures (e.g. the industrial application presented in Paper I) whereas for larger problems automated optimization is more time-efficient.

As pointed out in Section 3.2 and in Paper II, feasibility assessment (structural or general) only ensures feasibility but not energy efficiency or cost efficiency for different operating points. For this reason, it is necessary to include the evaluation of the performance at different representative operating points. In Paper II, a conservative estimation was done by considering the most extreme operating points (at maximum disturbance). In contrast to this conservative estimation, time-average values were chosen in Paper I and Paper III. Additionally, in Paper III these time-average values were weighted with their normalized duration factor (time period represented by operating point divided by entire time period). In general, the most extreme operating points are not representative. However, extreme operating points are straightforward to acquire once the expected disturbance range is defined (e.g. based on the most extreme variation occurring in historical data). For time-average values, time periods must be defined and theoretically there are infinitely many periods possible (seasonal, monthly, daily, etc.). In this context, different time-periods were chosen for Paper I (seasonal) and Paper III (monthly, with one month shut-down). Although the accuracy of a potential solution increases with increasing number of representative points, the size and thereby the complexity of the problem increases as well. Consequently, there is a trade-off between accuracy and complexity/computational load which needs to be balanced carefully.

In general, cost functions for retrofit problems are complex, highly dependent on the specific problem and difficult to derive. For this reason, simplified models are often used. An example can be found in Paper II. In Paper II, for the preliminary interpretation of the results of the feasibility assessment (design characteristics which achieve general feasibility), it was assumed that area increase would be penalized with the same investment cost factor of X €$/m^2_{increase}$. This makes it possible to compare different options directly from an investment cost perspective and the option with the smallest absolute increase was identified to be the most favorable one. However, this approach may be an invalid simplification since HEXs may be of different types which certainly results in different cost functions for area increase. Furthermore, there might be other limitations, e.g. spatial limitations which limit the increase of certain HEXs. In optimization problems, simplifications can be partly avoided if the retrofit measure is quantifiable by an appropriate cost function. However, complex cost functions (especially non-convex cost functions) usually lead to an exponential increase in computational load and increasing difficulty of finding feasible solutions. It should be noted that with the optimization-based approach presented in Paper III the even more difficult task of defining generic cost functions for different design changes was avoided by limiting the superstructure a priori to a selected number of design proposals.

In Paper III, difficulties were discussed which occurred when determining the critical points of the HEN example considered. In the Appendix A of Paper III, modifications were proposed to adapt the methodologies proposed by Pintarič and Kravanja [58] to determine critical points for the HEN example in question. However, further analysis is necessary to guarantee the validity of these proposed modifications also for other HEN examples. Additionally, in comparison to the HEN examples which have been used for critical point analysis and published in the literature (see [58, 61]), the areas of utility HEXs were not considered in Paper III. The reason for this is explained in Subsection 2.2.1 but a thorough analysis should be done to validate that not considering the areas of utility HEXs was not the reason for the difficulties occurred.

5
Conclusion

Since retrofitting of heat recovery systems is usually a difficult task, constrained by operability issues as well as size, type and location of existing equipment, retrofitting problems are usually very individual and easily reach high levels of complexity. A strategy presented in this thesis to cope with this complexity is to divide the retrofitting process into different sub-steps. In this way, it is possible to combine the beneficial designer interaction of graphical approaches (e.g. Pinch-based) at an early stage in the design process with the efficiency of mathematical programming to derive feasible and cost-efficient/energy-efficient retrofit measures. In this context, inefficient trial and error procedures are avoided. In general, different levels of division are possible together with different strategies. In this thesis, three different approaches have been developed.

Industrial heat recovery systems are often based on complex HENs. Regardless of the network complexity, HENs are usually based on similar sets of equations which implies that large parts of the modelling process can be automated. In this thesis, an automated HEN modelling strategy has been proposed which can be implemented in any high-level programming language. The modelling strategy can handle complexities commonly present in industrial HENs such as stream splits, closed loops or re-circulation. It is based on a table-based representation of the HEN which can be applied directly to a process flowsheet and a transformation to the commonly used but limited grid-diagram representation is not necessary. In addition to the implementation of the automated HEN modelling strategy in the computational analysis tool presented in Paper I, automated HEN modelling is of high interest for other advanced HEN analysis methodologies, e.g. feasibility analysis, energy performance analysis or critical point analysis.

With respect to feasibility analysis of HENs, the difference between structural and general feasibility has been defined. In this context, structural feasibility has been established as a premise for general feasibility. Furthermore, the approaches presented in Paper II and Paper III suggest different strategies to identify design modifications which achieve general feasibility with respect to a given objective, e.g. minimize external utility demand or minimize total annualized cost.

Furthermore, in addition to feasibility analysis, the need for energy performance analysis of HENs exposed to variations was identified to be able to fully compare different retrofit design proposals. Different strategies to allow a fair comparison between different design proposals were proposed, namely sensitivity analysis based on automatically derived sensitivity tables in Paper I, Energy Performance Ratios in Paper II and multi-period optimization in Paper III.

In comparison with the similarities of the proposed approaches, an interesting difference is the evaluation of the different retrofit proposals with respect to a certain objective. While the more manual approaches in Paper I and Paper II can be followed with rather vague and flexible objectives, the framework presented in Paper III requires a well-defined objective function. It should be noted that the selection of the approach is highly dependent on the overall (retrofitting) problem and the preferences of the designer.

The success of a HEN retrofitting project based on one of the proposed approaches depends to a large extent on the quantity and quality of the retrofit design proposals generated beforehand (by means of single-period retrofitting methodologies). A major limitation is that there is no certainty that the generated design proposals are structurally feasible. However, as outlined in Chapter 4, the definition of structurally feasible design proposals should generally be possible with some degree of iteration. In this context, the role and the experience of the designer must be stressed. Despite this limitation, by combining the existing variety of proven, single-period retrofitting methodologies with the approaches proposed in this thesis, it is likely that the adaptability of the developed retrofit design proposals can be substantially increased compared to design proposals derived with existing retrofitting methodologies presented in Section 1.1.

The approaches presented in this thesis yield opportunities to increase heat recovery in applications operating during multiple periods, e.g. industrial applications. In this context, increased heat recovery can contribute significantly to decarbonization of industry but also of other sectors, e.g. the heat supply sector if fossil-based heating is replaced by district heating from bio-based process plants. As decarbonization of all sectors is essential to limit the increase of the global average temperature well below 2 °C, systematic approaches to successfully retrofit industrial heat recovery systems are in demand more than ever. In comparison to existing approaches for retrofitting HENs operating in multiple periods, the approaches presented in this work divide the design process in sub-steps, which decreases the complexity of the sub-problems. The decreased complexity can be the decisive factor for a successful retrofit project when large and complex industrial applications are addressed.

6 Future Work

This chapter outlines some ideas for future work. These ideas are in different states which means that some ideas are developed further than others. The ideas proposed in this chapter arise partially from the issues presented in Chapter 4. This chapter focuses on the following four issues raised in Chapter 4:

- Problems occurring as a result of modifying operating constraints for the minimum temperature difference of HEXs (see Equations 2.4a and 2.4b as well as following paragraph in Subsection 2.2.1) when applying the active set approach to solve the flexibility index problem;
- Determination of representative operating points;
- Automatization of approaches discussed in Papers I and II; and
- Feasibility assessment considering correlations between different uncertain parameters.

In order to handle the proposed modified operating constraints to account for the dependency of these constraints on the HEX duty when solving the flexibility index problem by means of the active set approach, the mathematical formulation must be adapted. In this context, it must be ensured that the modified operating constraints are not identified (by the solver) to be part of the set of constraints which are active at the solution point if the corresponding HEX is bypassed (i.e. the duty of the corresponding HES is 0). Additional constraints in the form of logical expressions are necessary to ensure this. Disjunctive programming may be used to incorporate logical expressions in an optimization problem. Disjunctive programming was first introduced by Balas in 1979 [62] and has been continuously developed by a number of authors, e.g. Grossmann and Ruiz [63].

As determining representative operating points is based on historical data screening, an interesting alternative can be data-driven approaches. Recently, different strategies have been suggested in the literature to incorporate data-driven and especially clustering algorithms to identify representative operating points within time series data-sets (see, e.g. [64–68]). By means of data-driven clustering algorithms, clusters within data series can be identified which can then be used to define representative operating points. Additionally, there is the potential to decrease the workload necessary for data prepossessing (filtering, etc.) by means of, e.g. unsupervised clustering algorithms. Another advantage of clustering algorithms is that not only consecutive and isochronous (equally long) periods are considered. The pulp mill presented in Paper I can be named as one example since this mill runs both softwood and hardwood campaigns. As the hardwood campaigns have a typical duration of approximately one week per month, they would not be distinguished with monthly resolution and weekly resolution is necessary. However, since during most of the operating weeks softwood pulp is produced, evaluating each operating week with respect to the raw material may seem unreasonable. This could result in neglecting the different production campaigns by choosing, e.g. monthly average values. However, by utilizing clustering algorithms there is a good chance the different production campaigns would be identified which would allow dividing each month in two periods with respect to the raw material of the pulp.

In the context of data-driven approaches, there is commonly a significant amount of (historical) data available in process industry plants. Today this data is utilized either very little or not at all when analyzing operating decisions. This is also true for the optimization of these decisions. In this context, possible areas of application for data-driven approaches range from the optimization of operating parameters over the prediction for maintenance demand to the validation of operating decisions (e.g. a changed equipment cleaning routine).

Both approaches proposed in Papers I and II require hands-on work by the designer to a larger extent than the approach proposed in Paper III. More automatization is possible. For example, for the energy analysis step in Paper II, a tool can be developed with two objectives. Firstly, it needs to calculate the utility MER targets for predefined stream data sets (operating points) and, secondly, it needs to return the actual utility demand for these operating points given a HEN with specified network structure and heat exchanger areas. The first objective can be achieved by solving the minimum utility cost problem which was first introduced by Papoulias and Grossmann in the form of the transshipment model [69]. For the second objective, an optimization problem can be defined to manipulate the operational parameters of a HEN in such a way that the operational constraints are not violated while the external utility demand is optimized. In this context, a tool fulfilling the second objective can be used instead of sensitivity analyses to determine the optimal setting for the adjustable parameters discussed in Paper I.

Correlations between uncertain parameters are important to identify in order to avoid underestimation of the flexibility index. Additionally, these correlations should be considered during critical point analysis to avoid unnecessary oversizing of the equipment. Figure 6 (in Section 2.3) visualizes the flexibility index for two independent inlet temperatures of a HEN. If these two inlet temperatures are not independent but correlate in some way, different approaches to account for this are possible and will be investigated in future work. A brief overview is given below.

One way to express the correlations between inlet conditions is by expressing them in form of regression models, e.g. linear regression models. In this way, one or several inlet parameters are expressed as (linear) functions of the remaining (independent) inlet parameters. In the case of two correlating inlet temperatures of a HEN, one temperature can be expressed as a (linear) function of the other temperature. Consequently, the expected disturbance range cannot be visualized as a rectangle (as it was done for independent inlet temperatures in Figure 6), and the flexibility index δ cannot be expressed by Equations 2.10a and 2.10b. On the other hand, in the case of two correlating inlet temperatures, the flexibility index δ can be expressed by means of the following set of equations:

$$T_1 = f(T_2), \tag{6.1a}$$

$$T_{2,N} - \delta \cdot \Delta T_2^- \leq T_2 \leq T_{2,N} + \delta \cdot \Delta T_2^+. \tag{6.1b}$$

With respect to Equations 6.1a and 6.1b, for each value of T_2 , T_1 is defined by, e.g. a linear function. In Figure 11 this is visualized for two different example functions. The flexibility index can be interpreted as the minimum value for δ at which a combination of the uncertain parameters (here: T_1 and T_2) lies on the boundary of the feasible region. In accordance with this, the flexibility index has been marked for both example functions.

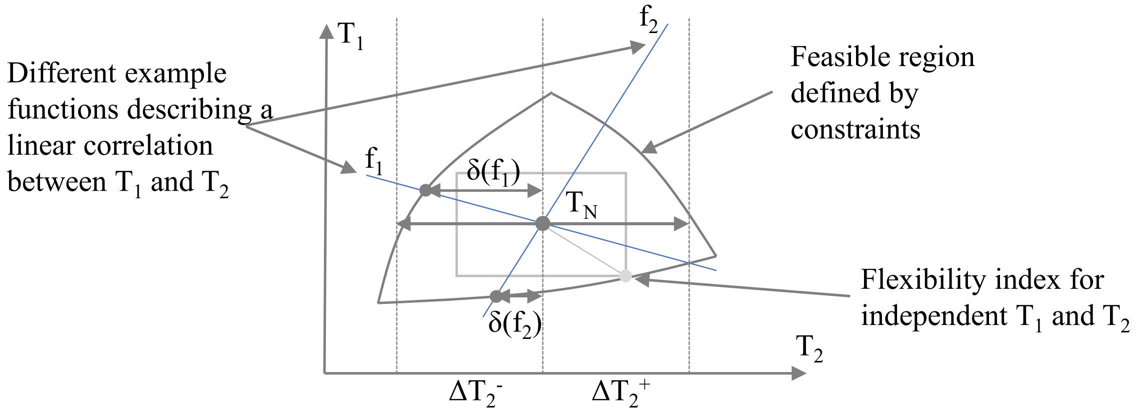


Figure 11: Visualization of the flexibility index for a heat exchanger network with two varying inlet temperatures which are correlated with a linear correlation; two example functions f_1 and f_2 are presented.

In the example shown in Figure 11, it is implied that the correlation between T_1 and T_2 can be described sufficiently by means of deterministic regression models. However, a good regression model represents per definition the majority of data points well while outliers are either neglected or weighted differently. Figure 12 shows the daily average values of two flow rates measured in the secondary heating system of a Swedish pulp mill. A linear correlation is shown which has reasonable properties ($R^2 = 0.8$). Additionally, in Figure 12 outliers can be identified which are not well represented by the linear regression model. This is critical if these outliers are crucial for operation. In order to include these outliers, instead of using the linear regression model to describe the flow rate shown on the y-axis (Fcp 1), Fcp 1 can be limited by a lower and an upper bound function. Consequently, the flexibility index can be described by the following set of equations:

$$f_l(T_2) \leq T_1 \leq f_u(T_2), \tag{6.2a}$$

$$T_{2,N} - \delta \cdot \Delta T_2^- \leq T_2 \leq T_{2,N} + \delta \cdot \Delta T_2^+. \tag{6.2b}$$

The lower and upper bound functions can be defined in order to include all points or only some points. An example of different upper bound functions is shown in Figure 12. The calculation of the flexibility index for such a case is visualized in Figure 13. Again, the flexibility index can be interpreted as the minimum value for δ at which a combination of the uncertain parameters (here: T_1 and T_2) lies on the boundary of the feasible region. This results in the marked point in Figure 13.

This idea for integrating correlations in feasibility assessment by means of lower and upper bound functions is highly conceptual. Future work is necessary to demonstrate general validity by applying the concept to case studies, among others. Additionally, the definition of lower and upper bound functions for problems with more than two mathematical dimensions and multi-variable correlations remains challenging at this stage.

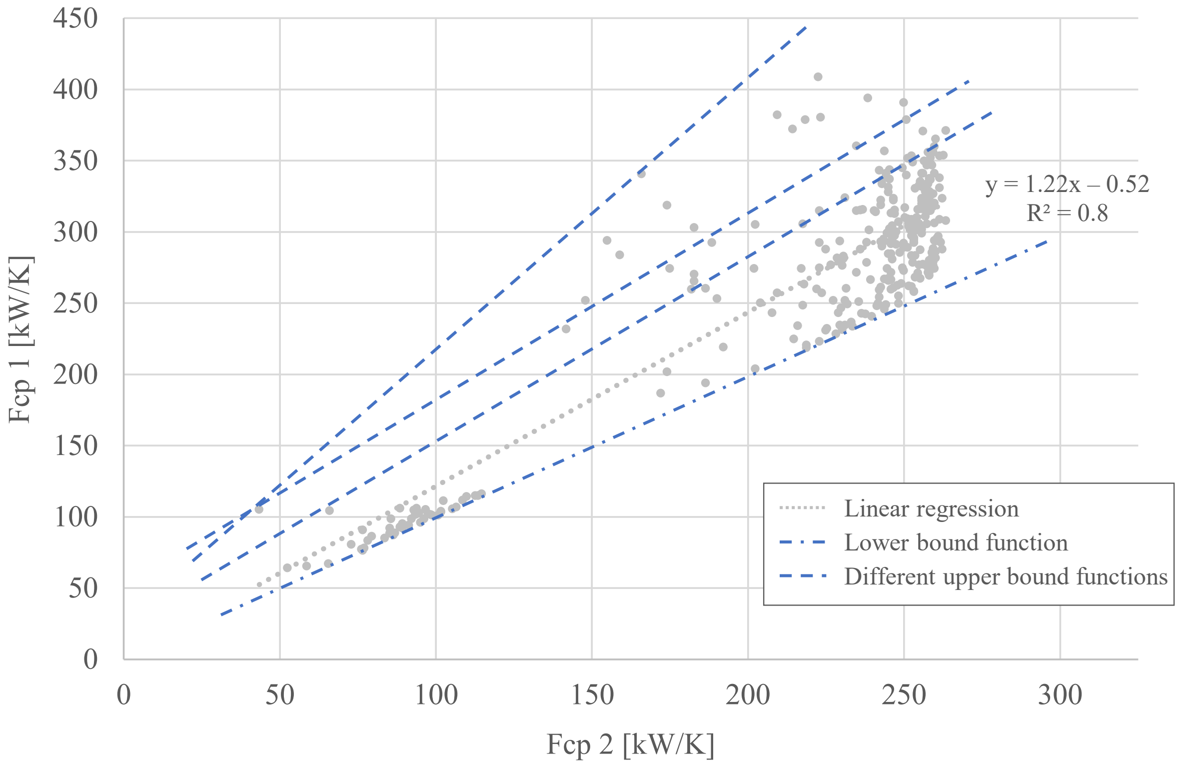


Figure 12: Correlation between two flow rates in the secondary heating system of a Swedish pulp mill; Visualization of one linear lower and three different upper bound functions to include outliers not captured by a conventional linear regression model.

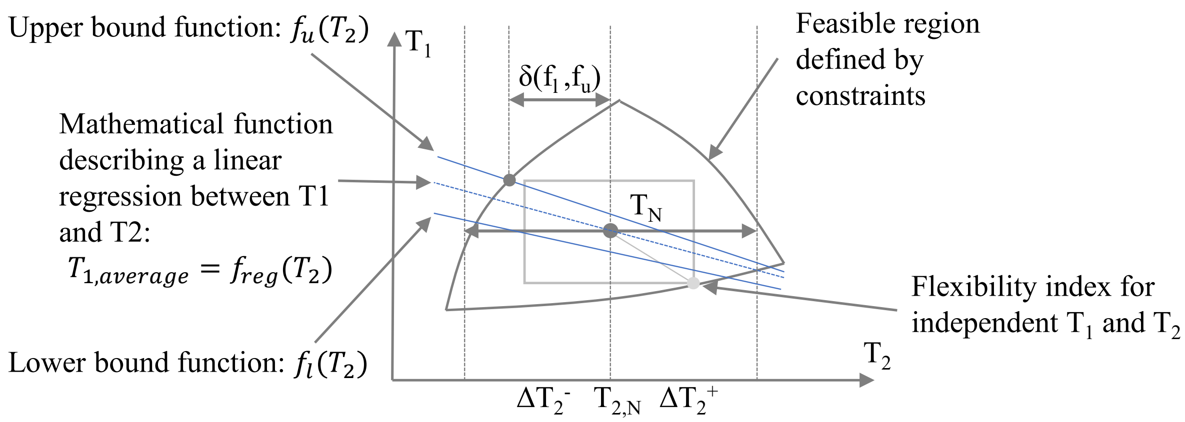


Figure 13: Visualization of the flexibility index for a heat exchanger network with two varying inlet temperatures which are correlated; the correlation is expressed by linear lower and upper bound functions.

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